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(54) PROCEDE D'ANALYSE DE METABOLITES
(54) METHOD FOR ANALYSING METABOLITES

(57)

Described is a method for analysing the metabolites of a biological sample which comprises quantitatively determining one or more metabolites in said sample in a way that said quantitative determination resolves isotopic mass differences within one metabolite, said method being characterized in that the sample comprises or is derived from a cell which has been maintained under conditions allowing the uptake of an isotopically labeled metabolizable compound so that the metabolites in said cell are saturated with the isotope with which said metabolizable compound is labeled. This method may further comprise, prior to quantitative determining the metabolites, combining the biological sample (i.e. the first biological sample) with a second biological sample in which the metabolites are not isotopically labeled or are isotopically labeled differently from the first biological sample; and determining in said biological samples the relative quantity of metabolites which differ by their isotopical label. Furthermore described is a set of isotopically labeled metabolites obtainable by applying this method, as well as kits facilitating the application of this method and corresponding uses.

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Method for analysing metabolites

The present application relates to a method for analysing the metabolites of a biological sample which comprises quantitatively determining one or more metabolites in said sample in a way that said quantitative determination resolves isotopic mass differences within one metabolite, said method being characterized in that the sample comprises or is derived from a cell which has been maintained under conditions allowing the uptake of an isotopically labeled metabolizable compound so that the metabolites in said cell are saturated with the isotope label. This method may further comprise, prior to quantitatively determining the metabolites, combining the biological sample (i.e. the first biological sample) with a second biological sample in which the metabolites are not isotopically labeled or are isotopically labeled differently from the first biological sample; and determining in said biological samples the relative quantity of metabolites which differ by their isotopical label. The present invention also relates to sets of isotopically labeled metabolites obtainable by applying this method, as well as to kits facilitating the application of this method and to corresponding uses.

The present invention belongs to the field of metabolome analyses, also referred to as metabolic profiling, i.e. the quantitative analyses of metabolites in a biological sample with the aim to investigate the state of organisms in particular with respect to biochemical regulatory networks. In the prior art, the metabolome, besides the proteome, transcriptome and genome, has become the fourth cornerstone of biological systems analyses. Only metabolome analyses allows insight into nutrient use, biosynthetic capacity of organisms, signalling and communication mediated via low molecular weight compounds and biochemical adaptive processes. Therefore profiling analyses of relative changes of all metabolites within an organism is in demand for a true biological systems analysis.

Metabolome analyses are still in early development inter alia because, in contrast to genome, transcriptome and proteome analyses, metabolome analyses has to deal with a highly diverse range of chemicals covering substances from small molecular

weight volatiles up to polymers. Conventionally, different and specialised analytical platforms are used in order to analyse these different classes of compounds. Meanwhile, universally applicable analytical platforms have been developed for complex mixtures of compounds. These exploit molecular mass and chromatographic retention in so-called hyphenated technologies, like GC-MS, HPLC-MS or MALDI-TOF. Bench-top gas chromatography coupled to mass spectrometry (GC-MS) was the first technology platform proposed for large-scale metabolome analyses (Trethewey, 1999). The choice of this hyphenated technology took into regard the ideal combination of unsurpassed chromatographic separation with high selectivity, sensitivity, and dynamic range of quantitative mass detection. Moreover, both GC and electron impact ionisation (EI) mass spectrometry exhibit only minor matrix effects as compared to other MS techniques, as for example matrix assisted laser desorption/ionisation-time of flight (MALDI-TOF) (Guo, 2002) mass spectrometry or liquid chromatography coupled to mass detection (HPLC-MS) (Matuszewski, 2003). High reproducibility of the GC-MS analyses of metabolites, which routinely uses methoxyamine hydrochloride (MEOX) and N-methyl-N-(trimethylsilyl)-trifluoroacetamide (MSTFA) reagents, allowed metabolite profiling based on external quantification of respective methoxyamine (MX) and trimethylsilyl (TMS) derivatives (Fiehn, 2000a; Roessner, 2000; Roessner, 2001). The scope of metabolites covered is, however, limited (1) by the required volatility of metabolites or stable chemical derivatives of unstable metabolites, and (2) by the distribution of metabolite concentrations within each type of sample. The maximum sample load of any multi-parallel chemical analyses is determined by the predominating metabolites. GC-MS metabolite profiles have an enormous dynamic range of 4 to 5 orders of magnitude. The upper limit of quantification is set by the requirement for surplus chemical reagent and by peak deformation effects due to chromatographic overloading. Thus, biological matrices devoid of single predominant metabolites promise best potential for highly complex multi-parallel analyses (Fiehn, 2000a; Roessner, 2000).

Two main strategies are conceivable toward a more comprehensive metabolome analyses: (1) the choice of other analytical techniques which may supplement GC-MS analyses, and (2) the application of pre-fractionation and concentration techniques for the enrichment of trace compounds. However, both strategies are currently highly limited. Supplementary MS techniques, as for example MALDI-TOF-

MS or HPLC-MS, are subject to strong interferences, which result from the changing compositions of complex biological matrices. These so-called matrix effects may lead even to complete suppression of ionisation and response signal (Matuszewski, 2003; Guo, 2002). On the other hand, most pre-fractionation and concentration techniques result in high or highly variable losses of metabolites.
These drawbacks preventing the use of potentially more powerful MS techniques in metabolite profiling studies may at least in part be overcome by including internal standards into the metabolite analyses. Indeed, a thorough quantitative standardisation for as many as possible measured metabolites is required. This would make it possible to extend the scope of metabolite profiling to such techniques, because it would allow an exact quantification of the metabolite levels for which a standard is available. From investigations on metabolic fluxes, it is known that metabolites can be labeled in vivo with a stable isotope (Wittmann, 2002). However, flux analyses are generally confined to the investigation of very limited biochemical pathways and do not cover metabolites in the breadth as is normally required for metabolic profiling. Consequently, the substrate compounds which are used in such studies in order to label cells with a stable isotope are typically very specific to the particular biochemical pathway to be analysed. Their production is expensive because it requires specific and time-consuming chemical syntheses.
To summarize, a practicable approach for establishing a quantitative standard for use in metabolite profiling is not in sight in the prior art. This is mainly explained by the diversity of compound classes to which metabolites may belong and by the fact that most of the metabolites cannot be tagged after extraction as it is possible for the chemically uniform transcripts and proteins (see, e.g., Gygi, 1999).

Thus, the technical problem underlying the present invention is the provision of means and methods that allow it to improve metabolome analyses by establishing a reliable quantitative standard for as many as possible metabolites in order to broaden the scope of such analyses.

This technical problem is solved by the provision of the embodiments as characterized in the claims.

Accordingly, the present invention relates to a method for analysing the metabolites of a biological sample which comprises quantitatively determining one or more metabolites in said sample in a way that said quantitative determination resolves isotopic mass differences within one metabolite, said method being characterized in that the sample comprises or is derived from a cell which has been maintained under conditions allowing the uptake of an isotopically labeled metabolizable compound so that the metabolites in said cell are saturated with the isotope with which said metabolizable compound is labeled.

The present invention is based on the experiments described in the appended Examples which show that it is possible to label substantially all possible metabolites in vivo. The proof that this principle works has been obtained by labeling yeast cells with U-^{13}C-glucose. This work represents the keystone to comprehensive, fully quantitative metabolome profiling and will greatly facilitate future developments within this field. It solved the technical problem of standardisation by differential labeling of metabolites with isotopes. Similar to differential labeling of transcript samples by fluorescent probes or of protein samples by chemical tagging, it is possible in the method of the present invention to tag the metabolome by saturating in-vivo labeling with isotopes. This concept can be extensively exploited for a non-biased sampling of mass spectral metabolite tags (MSTs) and isotopomer ratio (ITR) metabolite profiling. In particular, isotope-saturated extracts produced by the method of the invention may be used as a multiplex mixture of internal standards, where each component of the resulting metabolite profiles will be quantified relative to the respective fully labeled isotopomer (see Example 4 and Figure 2). It is envisaged that these achievements, in particular the compilation of a first compendium of MSTs which, analogous to ESTs, allows qualitative assessment of the metabolome composition and the demonstration of fully quantitative ITR metabolite profiling, will greatly improve metabolome analyses.

In the prior art, isotope labeling studies are routine approaches used for metabolite flux analyses (Wittmann, 2002; Christensen (1999); Wiechert, 2001. These studies require isotopically labeled compounds, which are expensive and of limited availability. In a conventional flux experiment, a labeled compound is fed to

organisms, which are pre-grown on media with ambient isotope distribution (dos Santos, 2003; Lee, 1991) resulting in the labeling of a corresponding specific isotopically labeled metabolizable compound. However, flux studies differ from the method of the invention in that they generally involve partial labeling of the metabolites of a cell. This is explained by the fact that flux studies require partial, i.e. incomplete, labeling. By contrast, the method of the present invention achieves saturating labeling which means a labeling of the metabolites as complete as possible given the degree of labeling in the isotopically labeled metabolizable compound used to label the cell from which the biological sample for analyses is derived (for more detailed definitions see below).

One advantage of the present method is the fact that it introduces an isotopic label at the site which is ideal for metabolome analyses, namely the active biological sample. In prior art technologies, a differential label is often introduced only in the course of chemical analyses such as in the currently prevailing methods for quantitative proteome (Aebersold, 2003) and transcriptome (Duggan, 1999) analyses. These technologies for example involve isotope-coded protein-tagging techniques (Gygi, 1999) and two-colour labeling by fluorescent probes (Schena, 1995; Lockhart, 1996). However, labeling only after extracting the respective compounds from the cell may introduce a bias in the labeling result. Such artefacts are excluded in the method of the invention.

Apart from incorporation of label in the course of chemical analyses, there has been at least one approach to label proteins in vivo. Oda (Proc. Natl. Acad. Sci. USA 96 (1999), 6591-6596) describe whole cell-labeling for proteome analyses using the stable isotope ^{15}N. However, in vivo isotope labeling of the entire set of metabolites has not been reported in the prior art. In particular, by using ^{13}C-labeling of yeast cultures, the present invention demonstrates that combined mass spectral analyses of differentially labeled samples, especially ^{13}C-ITR profiles, can be generated. In particular, the experiments underlying the present invention surprisingly show that complete (i.e. saturating) labeling of metabolites could be achieved in yeast cells. The results obtained in the appended Examples are surprising because it could not have been excluded that carbon sources other than the isotopically labeled metabolizable compound (in the examples U-^{13}C-glucose) which are present in the medium could have prevented an efficient broad isotope labeling of the metabolites.

It is almost impossible to avoid in the medium the presence of such other carbon sources like for instance essential nutrients, such as vitamins, or auxotrophic markers. The processing of these compounds in the cultured cells could have severely interfered with isotope labeling and thereby prevented the required saturating labeling. However, as is shown in the Example experiments, the lack of labeling in the cell due to the presence of the unlabeled carbon sources in the medium is greatly restricted to the compounds themselves or to direct metabolic products thereof (see Example 1). A mixing of label with unlabeled compounds essentially did not take place. This was surprising and means that in vivo labeling with isotopes can indeed be applied for achieving broad coverage of the metabolites with isotopic labeling.

Another surprising finding was that the presence of isotope label in the metabolites does not substantially influence the distribution of metabolite levels in the sample when it is compared with a metabolite profile obtained from a corresponding unlabeled sample (i.e. a sample, wherein the cells have been fed with nutrients in which the isotopes are present in the naturally occurring, i.e. ambient proportions). This is for example evident from the results depicted in Figure 2 and described in Example 4. This could not have been expected since it is known that enzymes may discriminate between isotopomers. For instance, such effects are described from plant physiology such as for RUBISCO, CO_2-fixation and phosphoenolpyruvate carboxylase (PEPC) (see, e.g., Le Roux-Swarthout, J. Plant Physiol. 157 (2000), 489-493) and from fungi, yeast or other microorganisms, e.g., for pyruvate decarboxylase (PDC), and the isoprenoid metabolizm (see, e.g., Stivers, Biochem. 32 (1993), 13472-13482; Henn, Appl. Environ. Microbiol. 66 (2000) 4180-4186; Londry, Appl. Environ. Microbiol. 69 (2003), 2942-2949). Thus, it was reasonable to expect that, caused by isotope discrimination, the labeling of metabolites with isotopes would influence the distribution of metabolite levels in the biological sample. But, as it is shown herein, the isotopically labeled metabolites show a distribution that greatly corresponds to that obtained for unlabeled metabolites. This proves suitability of the method of the invention for standardizing metabolite analyses.

The experimental results summarized in the following show that the method of the invention may become an indispensable tool for the future development of metabolite profiling.

The present invention is herein exemplified in experiments using a Saccharomyces cerevisiae model which was subjected to saturating in vivo stable isotope labeling by growing on an exclusive ^{13}C-source (see, e.g., Figures 1 and 9). The in vivo labeling of metabolites in yeast generates isotopomer tags which could be differentially detected by mass spectrometry. When applied as internal quantitative standard, isotope-labeled compounds may facilitate a meaningful quantitative analyses if for example two samples, the one being saturatingly labeled and the other not being labeled (i.e. having ambient isotope abundances) are compared and the relative ratio between each isotopomer tag and the corresponding unlabeled metabolite is determined. Interestingly, this working principle may even facilitate those mass spectral technologies such as MALDI-TOF-MS which are prone to matrix suppression effects and high variability and which therefore hitherto were not applied for quantitative metabolite profiling analyses. An example of successfully using the method of the invention by applying MALDI-TOF-MS is presented herein (Example 9 and Figure 9). This means that the method described herein may allow to extend multi-parallel metabolite profiling in principle at least to all mass spectrometry-based technologies.

A further advantage of the method of the invention over conventional metabolome analyses is that it allows an immediate proof of the metabolic origin of any mass spectral tag which is detected in biological samples. While protein and mRNA sequence diversity provides information about the source species by the sequence information contained therein, the origin is not immanent in metabolite structure per se, except for the subset of species-specific secondary metabolites. However, as soon as a pair of labeled and non-labeled MSTs is found, chemical artefacts or laboratory contaminations can immediately be ruled out.

In addition, mass shifts allow a direct insight into the number of carbon atoms present within each compound or fragment. This property of the method of the invention increases the insight into the chemistry of those MSTs the chemical nature of which is unknown and may support the identification of MSTs by other techniques (Table 3).

In analogy to expressed sequence tags (ESTs), identified and non-identified MSTs may be used as a highly useful tool to characterise the metabolome of any biological sample. Again in analogy to tools for sequence comparison, MSTs can easily be

identified by matching of mass spectral fragmentation and chromatographic retention. Furthermore, clustering technologies allow a meaningful classification of MSTs (Figure 4) (Wagner, 2003).

As a further advantageous property, the method of the invention allows a fast investigation of the precision of analytical methods which are being developed for metabolite profiling. In addition, it makes quantitatively standardized metabolome analyses accessible to biological samples which are obtained by pre-purification and enrichment of fractions of the total metabolite extract taken from a biological sample, for instance in order to detect trace metabolites. In the prior art, such samples fall below the detection limits of conventional GC-MS profiling. The possibility of the method of the invention to quantitatively determine minor amounts of metabolites facilitates to conduct metabolite co-response analyses which may provide direct information about quantitative metabolite interactions in biological systems. Such interactions may be expected based on theoretical considerations (Steuer, 2003). Observed metabolite co-responses may be uncoupled or may follow linear functions. Metabolite co-response may be either constitutive or conditional with respect to the set of experiments under investigation. In Example 8, metabolite co-response analyses applying the method of the invention are described. Accordingly, metabolite co-responses may best be discovered and judged by a set of different distance measures, among which the Euclidian distance is least indicative (Figure 6). Metabolite interactions may reflect canonical pathway definitions (Figure 7), but may also allow to discover cross-pathway interactions (Figure 8). Investigations into these interactions are highly valuable, because they can provide insights into common mechanisms of metabolic control. However, to date, such analyses are restricted due to the limited coverage of metabolome data. Based on the extension of metabolite data mining that is now possible by applying the method of the invention, for instance because of the possibility to exploit MALDI-TOF for quantitative determination of metabolite levels on a broad scale, it is conceivable that the present invention will further the development of quantitative metabolome analyses, in particular towards trace compounds and general co-factors.

As it is explained above, the present invention belongs to the field of the metabolic profiling or metabolome analyses. This means that the method of the invention is of use for quantitatively determining one or more metabolites in a biological sample.
The term "quantitative determining" refers to the determination of the relative or absolute amount of each analyzed metabolite in the sample. Generally, such a determination leads to a so-called metabolite profile pertaining to the respective biological sample. Such metabolite profiling approaches have been carried out in many laboratories and therefore belong to the prior art.
Since isotopic labeling is applied in the method of the invention, it is necessary that the technique used to quantitatively determine the metabolites resolves isotopic mass differences as they may occur within one metabolite. Compounds that differ from one another only by one or more isotopes incorporated into the chemical structure are generally referred to as "isotopomers". The technique used to detect the metabolites must therefore be capable of discriminating between two compounds that differ in their mass by as little as one relative atomic mass. Corresponding techniques are known to the skilled practitioner and described in the literature. They involve different kinds of mass spectrometry or NMR, as is described in further detail further below.
The term "isotopic labeling" is to be understood to refer to compounds that are labeled with an isotope that is not the main isotope of the element of said isotope. "Labeled" means in this context to have a significantly and, for detection purposes, usefully increased proportion of the label-isotope as compared to the abundance of said isotope occurring in nature, preferably the proportion of the label-isotope is increased to at least 80%, more preferably to at least 90% and even more preferably to at least 95% and most preferred to at least 99% of the total of all isotopes of the respective element. The term "isotopic labeling" furthermore preferentially refers to compounds in which the label-isotope is present in the above-mentioned proportion at each possible position within the chemical structure of the compound. However, partial labeling of compounds may also be of use in the context of the present invention. Such applications require that means of correction for the proportion of residual non-labeled isotopomers are applied. In this case, labeling needs to be saturating, i.e. the proportions of isotopomers for each metabolite needs to be constant in the labeled sample, so that the isotopomer proportions can be

determined in a control experiment and used for mathematical correction of the metabolite profiling results. Preferably, the isotopically labeled metabolizable compound used in order to label the cell contains of the respective element only the label-isotope (in the proportion that is technically feasible) as it is the case with U-^{13}C-glucose where all six carbon atoms are the ^{13}C isotope.

The method of the present invention is characterized in that the sample comprises or is derived from a cell which has been maintained under conditions allowing the uptake of an isotopically labeled metabolizable compound so that the metabolites in said cell are saturated with the isotope with which said metabolizable compound is labeled.

It is a critical feature of the method of the invention that the metabolites are saturated with the isotopic labeling. "Saturated" (or "saturating labeling") means that the metabolites in the cell or the biological sample derived therefrom contain an amount of isotope label that substantially corresponds to the amount of label in the metabolizable compound taken up by the cell in order to label it, and that substantially all of the metabolites to be analyzed contain the isotope label. In particular, "saturating labeling" refers to an amount of labeling of the metabolites to be analyzed so that these metabolites overall contain at least 50%, preferably at least 70%, more preferably at least 80%, still more preferably at least 90% and most preferably at least 95% of the amount of isotopic label as present in the isotopically labeled metabolizable compound. The term "substantially all of the metabolites to be analyzed contain the isotope label" means that at least 70%, preferably at least 80%, more preferably at least 90%, still more preferably at least 95% and most preferably at least 98% of the metabolites to be analyzed are labeled, i.e. differ by at least one relative atomic mass from the corresponding unlabeled counterpart. Preferably, substantially all of the metabolites to be analyzed contain the isotope label if at least 20, more preferably at least 50, still more preferably at least 100, even more preferably at least 150 and most preferably at least 200 or even at least 300 metabolites of the biological sample to be analyzed contain the isotopic label.

Exceptions to the labeling to saturation may be tolerated, however, should be taken into account when analysing the metabolite data obtained. Non-labeled metabolites may be present in the biological sample when, in addition to the isotopically labeled metabolizable compound, other compounds, for example essential nutrients like

metabolizable compound, other compounds, for example essential nutrients like vitamins or auxotrophy markers, have been provided to the cell via the culture medium and these compounds do not contain the isotope label. Therefore, it may happen that cells which are labeled to saturation contain unlabeled metabolites which are these other compounds or metabolic products thereof.
The number and selection of metabolites analyzed in the method of the invention depends on the goal to be achieved by carrying out the method of the invention. It is typical for metabolic profiling like the method of the invention to aim at quantitatively determining an as large as possible subset of metabolites in order to obtain as much as possible metabolite data. Here, the possibility to label in principle each metabolite by the method of the invention is a big advantage over prior art approaches because it provides a quantitative standard for each metabolite to be analyzed.

Accordingly, in a preferred embodiment of the method of the invention, at least 20, more preferably at least 50, still more preferably at least 100, even more preferably at least 150 and most preferably at least 200 or even at least 300 metabolites are quantitatively determined.

The term "metabolite" refers to any substance within a cell or produced by a cell, including secreted substances, which can be quantitatively determined by applying the method of the invention, that is for which suitable techniques for determining the amount are available. Preferably, these substances are not macromolecules (i.e. biopolymers) such as DNA, RNA or proteins. Particularly preferred are metabolites with a low molecular weight preferably the metabolites have a molecular weight of not more than 4000 Da, preferably not more than 2000 Da, more preferably not more than 1000 Da. Typically, the metabolites to be analyzed may belong to the following, non-limiting list of compounds: carbohydrates (e.g. sugars, oligo- and polysaccharides such as polyglucans as for example starch or polyfructans), sugar alcohols, amines, polyamines, amino alcohols, aliphatics, aliphatic alcohols, amino acids, lipids, fatty acids, fatty alcohols, organic acids, organic phosphates, organic ions, other inorganic ions bound to metabolites, nucleosides, nucleotides, sugar nucleotides, purines, pyrimidines, such as adenine and uracil, sterols, terpenes, terpenoids, flavons and flavonoids, glucosides, carotenes, carotenoids, cofactors,

ascorbate, tocopherol, vitamins, polyols, organic amines and amides such as ethanol amine and urea and/or heterocyclic compounds such as nicotinic acid.
As is evident from the appended Examples, the method of the invention also involves analysing metabolites of which the chemical nature is unknown. However, metabolites (herein also referred to as "mass spectral metabolite tags" or "MSTs") of unknown chemical nature may nevertheless provide informative data on the biological sample analysed. It is clear that, if a metabolite of unknown chemical nature is revealed by carrying out the method of the invention to have an interesting property or diagnostic value or characteristic behaviour, this metabolite may be further characterized by applying suitable analytical methods known in the art.

In a particularly preferred embodiment, the method of the invention refers to the quantitative determination of metabolites comprising sugars, sugar alcohols, organic acids, amino acids, fatty acids, vitamins, sterols, organic phosphates, polyamines, polyols, nucleosides, purines, pyrimidines, adenine, uracil, organic amines and amides such as ethanol amine and urea and/or heterocyclic compounds such as nicotinic acid.

The isotope used for in vivo labeling in connection with the present invention may be selected among available isotopes that may be suitable for applying the method of the invention. As a preferred selection, a skilled person may use an isotope for which corresponding isotopically labeled metabolizable compounds are available, in particular commercially available. As a further preferred choice, isotopes for use in the method of the invention should be such that they do not harm viability of the cells from which the biologically sample for analyses is taken or that they do not interfere with the metabolizm such as by influencing the activity of metabolic enzymes. In this regard, it is thus preferred to use stable isotopes rather than radioactive ones. As a further aspect, one should take into account that elements such as carbon or hydrogen are preferred over elements that are present in metabolites more rarely in order to cover the metabolites of a cell by in vivo labeling as completely as possible. Particularly preferred isotopes are ^{13}C, ^{15}N, ^{18}O and ^{2}H, with particular preference of ^{13}C.

The label-isotope is incorporated into the cells from which the biological sample for analyses is taken by maintaining the cell under conditions allowing the uptake of said compound. This means that the compound should be one that is readily taken up by the cells and that is also readily metabolized so that it is ensured that saturation with the isotopic label can be achieved. Depending on the kind of cells or organism to be labeled, the label may for example be provided by feeding cultured cells such as yeast cells or mammalian cells with a nutrient, e.g. a carbon source if the label is ^{13}C. If the cells to be labeled are within a multicellular organism, the label may be incorporated by subjecting the labeled metabolizable compound through the substrate (e.g. the water) if it is a plant or by injecting the labeled compound into it if the organism is an animal, for instance a vertebrate, in particular a mammal.
As the isotopically labeled metabolizable compound, substances should be used that provide for an effective uptake of the label by the cell. Preferably, the compound may be totally labeled with the isotope (i.e. no atom of the respective element in the compound is of another isotope than the label-isotope). Corresponding labeled compounds may be available from commercial suppliers such as those mentioned in the Examples. Particularly preferred isotopically labeled metabolizable compounds are U-^{13}C-glucose, $^{2}H_2O$, $H_2{}^{18}O$, U-^{13}C acidic acid, ^{13}C carbonate and ^{13}C carbonic acid.

The term "biological sample" encompasses any amount of material comprising cells or derived from a cell that is susceptible to the method of the invention. In the present context, the term "cell" refers to any conceivable living entity that is capable of being in vivo-labeled according to the teachings of the present invention. Accordingly, the method may be applied to any type of cell, prokaryotic or eukaryotic cells, viral particles, wild-type or transformed, transduced or fused cells, or derivatives thereof such as membrane preparations, liposomes and the like. The cells may furthermore be part of a tissue, an organ or a complete organism such as a plant or an animal. The cells may be in a naturally occurring form or in a man-made form such as in a cultured form, e.g. cell culture, protoplast culture, tissue culture or the like.
The term "derived" used in connection with characterizing the biological sample means any kind of measures a skilled person may apply in order to modify the labeled cells or the direct environment of the cells, wherein the "direct environment"

is characterized by the presence of at least one metabolite produced by the cells, in order to prepare a sample for use in quantitatively determining the metabolites contained therein by applying the method of the invention. Such measures may for example involve typical sample preparation or extraction techniques common to those skilled in the art. The direct environment may for example be the extracellular space around a cell, the apoplast, the cell wall, the interstitial space or the culture medium. Furthermore, the biological sample derived from a cell may be a certain part of the cell, for example certain cellular compartments such as plastids, mitochondria, the nucleus, vacuoles etc. In a preferred embodiment of the present invention, the biological sample comprises yeast cells or plant cells.

A "biological sample" in the context of the present invention can for instance be fresh material such as a tissue explant, a body fluid or an aliquot from a bacterial or cell culture, preferably deprived of the culture medium, that may be directly subjected to extraction. On the other hand, samples may also be stored for a certain time period, preferably in a form that prevents degradation of the metabolites in the sample. For this purpose, the sample may be frozen, for instance in liquid nitrogen, or lyophilized.

The samples may be prepared according to methods known to the person skilled in the art and as described in the literature. In particular, the preparation should be carried out in a way suitable to the respective detection technique applied. Furthermore, care should be taken that the respective compounds to be analyzed are not degraded during the extraction process. Biological samples for metabolite analyses may for example be prepared according to procedures described in Roessner (2000).

In a further preferred embodiment, the method of the invention further comprises fractionating or purifying the biological sample so that the sample contains a subset of the metabolites contained in the cell from which the sample is derived.

By this additional fractionation and/or purification step, it is for example possible to select low abundant metabolites out of the whole pool of metabolites whereby, without this step, these metabolites might not be detectable for example because their signals are superimposed with strong signals of highly abundant metabolites. In prior art metabolite profiling methods, such a fractionation or purification would cause the loss of the quantitative relationship to other metabolites which would render the

quantification of low abundant metabolites nearly impossible. This problem has been overcome by the present invention since the isotopically labeled metabolites serve as a quantitative standard that may be co-fractionated/-purified with the non-labeled metabolites.

The fractionation and/or purification may be carried out according to standard procedures known in the art. It is clear that preferably procedures should be used that do not or at least only to a low tolerable degree change the distribution of the metabolites in the sample.

The quantitative determination of metabolites in a biological sample may be carried out by any known suitable method that can resolve mass differences within one metabolite. This may involve various nuclear magnet resonance (NMR) and mass spectrometry (MS) techniques that are known to a person skilled in the art, whereby mass spectrometry is preferred in the context of the present invention. Different suitable NMR and MS techniques are for instance described in Wittmann (Adv. Biochem. Engin. Biotechnol. 74 (2002), 39-64) and Szyperski (Q. Rev. Biophys. 31 (1998), 41-106). Preferred set ups for MS techniques for use in the present invention involve the combination of MS with gas chromatography (GC) as it is routinely used in state-of-the-art metabolite analyses, such as GC-MS described in the appended Examples.

In cases of ambiguous fragment interpretation, analyses using GC-MS-MS or corresponding MS tandem arrangements may support the identification of isotopomer fragment pairs. For example, GC-MS systems supplied with ion trap technology allow the selection of individual primary fragments and subsequent secondary mass spectral fragmentation (Birkemeyer, 2003; Mueller, 2002). These MS-MS mass spectral fingerprints may allow an unequivocal identification of corresponding primary ions.

The determination of the amount of metabolites of interest can be done according to well-known techniques known in the prior art and familiar to the person skilled in the art. Preferably, techniques are applied that allow the identification and quantification in one step and, advantageously, are suited to record the respective metabolites contained in the sample in a comprehensive manner.

Further methods for quantitatively determining the metabolites for use in accordance in the present invention include liquid chromatography/mass spectrometry (LC/MS), the use of radioactivity in connection with suitable methods known to the skilled person, thin layer chromatography (TLC), capillary electrophoresis (CE), direct injection MS, flow injection MS, MS/MS, MS/MS/MS, and further combinations of MS steps (MSn), fourier transform ion mass spectrometry (FT/MS), gel permeation chromatography (GPC), TLC, CE, HPLC, GPC, any other chromatographic or electrophoretic technique or any mass spectrometric technique which is hyphenated in-line or off-line to mass spectrometry. If appropriate, any of the above methods may be combined.

An exemplary non-biased analyses is described in Fiehn (2000b). In this study, of different plant mutants, 326 distinct compounds (ranging from primary polar metabolites to sterols) were detected and relatively quantified, including both identified and non-identified compounds, by applying GC/MS analyses. Another example of a GC/MS analyses that can be applied in the method of the invention has been described by Roessner (2001), where it was used for comprehensively studying the metabolizm in potato tubers.

In a particularly preferred embodiment of the method of the invention, the mass spectrometry used is matrix-assisted laser desorption ionisation/time-of-flight (MALDI-TOF) mass spectrometry.

This embodiment makes use of the surprising finding that the saturating in vivo labeling achieved by the method of the invention makes it possible to obtain quantitative metabolite profile data.

It is furthermore preferred that the method of the invention as described hereinabove involves that the metabolites are chromatographically separated prior to quantitative determination.

This preferred embodiment refers to the chromatographic separation which has already been described above by referring to the particularly preferred example of using gas chromatography in settings such as GC-MS or GC-MS-MS. Other suitable chromatography methods such as HPLC, RP-HPLC, ion-exchange HPLC, GPC, capillary electrophoresis, electrophoresis, TLC, chip-base micro-fluidic separation,

affinity-interaction chromatography using antibodies or other ligand-specific binding domains may also be used in this regard.

In another preferred embodiment, the method of the invention further comprises the step of introducing external standards for one or more of the quantitatively determined metabolites.
The introduction of external standards or standard dilution series allows the determination of metabolite concentrations in absolute terms. By contrast, embodiments of the method of the invention in which no external standards or standard dilution series are applied allow the exact quantification in relative terms, i.e. concentration changes observed relative to reference quantities as observed in experimental control samples. The introduction of external standards and the provision of such standards may be carried out as described in the literature and as is known by the person skilled in the art.

As has been mentioned above, the method of the invention includes the quantitative determination of metabolites the chemical nature of which is yet unknown. Accordingly, in a preferred embodiment, this method further comprises the step of identifying one or more of the metabolites which are quantitatively determined.
This identification may be carried out by analytical methods known to the skilled practitioner and described in the literature.

In a particularly preferred embodiment, this identification comprises identification by secondary fragmentation.
Secondary fragmentation techniques may be carried out by methods known in the prior art, in particular by GC-MS-MS or other MS^n techniques. Separate recording and subsequent comparison of chemical intermediates from MS-MS fragmentation pathways of, e.g., ^{13}C isotopomer pairs is highly facilitated by providing the number of carbon atoms present within each observed MS-MS fragment.

In an especially preferred form of this embodiment, identification of the metabolites comprises electron impact ionisation, MS-MS technology and/or post source decay analyses of molecular ions or fragments.

Such techniques are known to a person skilled in the art. In particular, post source decay analyses may be carried out as is described in Example 9 using NADH detection as an example.

In a further preferred embodiment, the method of the invention as described above may be carried out in such a way that the cell to be labeled has been maintained under conditions additionally allowing the uptake of an isotopically unlabeled metabolizable compound and said compound and/or metabolic products thereof are quantitatively determined. Preferably, the uptake of the unlabeled compound takes place when the cell is already saturated with the isotopic label.

Preferably, this embodiment involves comparing the amount determined for the isotopically unlabeled metabolizable compound and/or said metabolic products thereof with the amount obtained by carrying out said method correspondingly, but without the uptake of said unlabeled metabolizable compound.

The present preferred embodiment relates to an application of the present invention which is also referred to as "inverse labeling". This term refers to an inversion of conventional flux studies (see, e.g., Wittmann, Adv. Biochem. Engin. Biotechnol. 74 (2002), 39-64) in which a labeled metabolite is added to a cell and its fate is traced in order to analyse metabolic pathways. The present preferred embodiment of the invention appears to be feasible because of the high similarity of metabolite profiles from ambient $\delta^{13}C$- and ^{13}C-saturated yeast cultures (Figure 2 A, B). Moreover, in Example 2, a corresponding experiment is described in which L-lysine was added in unlabeled form to the culture medium after the yeast cells reached saturated ^{13}C-labeling. In a further experiment, the enrichment of the non-labeled trace compound nicotinic acid and the incorporation of this moiety into NAD(H) within a ^{13}C-saturated yeast metabolome was shown (Example 9).

The present embodiment allows it to achieve results similar to those obtained in conventional flux studies. It allows to utilize the relatively inexpensive supply of substances with ambient $\delta^{13}C$ composition for biochemical pathway elucidation within the background of a ^{13}C-saturated metabolome. But it has the advantage that the specific metabolite the metabolization of which shall be analysed does not need to be provided in labeled form, which often is considerably expensive. Rather, in the method according to the present embodiment, the metabolite to be investigated can

be used in the cheaper unlabeled form. A further advantage is the increased versatility of this approach as compared to conventional flux studies since virtually every possible metabolite can be tested for or even more than one metabolite, without being dependent on the availability of the metabolite(s) in labeled form.

In a further preferred embodiment of the above-described method of the invention, one or more proteins and/or transcripts in said sample(s) is/are quantitatively determined and analysed, in addition to metabolites.
This embodiment refers to one of the main aspects in systems biology which aims at combining metabolome data with data obtained from transcriptome and/or proteome analyses in order to obtain a comprehensive picture of regulatory mechanisms in biological systems. In this context, it is evident that the method of the present invention may be combined with methods that quantitatively determine transcripts and/or proteins from the same biological system, in particular organism or cells, of which the metabolites are quantitatively analysed in accordance with the method of the invention. Transcriptome and proteome analyses as well as mathematical evaluation and correlation analyses of the data may be conducted by methods described in the prior art. It is contemplated that, preferably, the transcriptome and/or proteome analyses conducted in combination with the metabolome analyses according to the present invention may also benefit from the advantages of in vivo labeling. Thus, if the quantitative determination of transcripts or proteins is done by suitable techniques such as mass spectrometry the transcripts or proteins may be isotopically labeled just as the metabolites and thereby also be used as a quantitative standard.

It is particularly preferred that the preferred embodiment is carried out in such a manner that said metabolites and proteins and/or transcripts are each determined from the same biological sample.
This particularly preferred embodiment is based on a technology described in WO 03/058238 and in Fiehn (Eur. J. Biochem. 270 (2003), 579-588). The method described therein provides data useful for quantitatively analyzing metabolites, proteins and/or RNA in a biological source material, whereby said analyses involves suitable statistical evaluation and correlation analyses on the data obtained. In this

method, extracting, identifying and quantifying of at least two compound classes of the group consisting of metabolites, proteins and RNA are each determined from one sample. Accordingly, in the present particularly preferred embodiment, the sample preparation in order to quantitatively determine metabolites and proteins and/or transcripts is carried out by applying the corresponding teachings of WO 03/058238. Thereby, it is especially preferred that (i) the metabolites are extracted from the sample with at least one solvent or mixture of solvents; and (ii) the RNA is extracted from the remainder of the sample after step (i). Thereby, it is a further option that metabolites may additionally be extracted from the yet undissolved remaining cellular material contained in the sample after step (ii). Preferably, extraction is carried out by using a mixture of solvents that comprises at least one highly polar solvent, at least one less polar solvent and at least one lipophilic solvent, advantageously a mixture of solvents comprising water, methanol and chloroform. More preferably, this mixture of solvents contains water, methanol and chloroform in the approximate proportion by volume of 1: 2.5: 1. Advantageously, the extraction in step (i) is carried out at a temperature between -60°C and +4°C.

As a further preferred embodiment of the present invention, the method as described hereinabove further comprises, prior to quantitative determining the metabolites, combining the biological sample (i.e. the first biological sample) with a second biological sample in which the metabolites are not isotopically labeled or are isotopically labeled differently from the first biological sample; and determining in said biological samples the relative quantity of metabolites which differ by their isotopical label.
Preferably, the second biological sample is not isotopically labeled.
By this preferred embodiment, the method facilitates the quantification of metabolite data which hitherto was only possible by using external metabolite samples as quantitative standards. Here, the in vivo labeled metabolites present the quantitative standard for the metabolites of the second biological sample. This allows the correlation analyses of a wide set of metabolites of two biological samples which correspond to two different phenotypic and/or genotypic states of the cells from which the biological samples are derived.

Accordingly, in a specifically preferred embodiment, the first and the second biological sample correspond to different phenotypic and/or genotypic states of the cells comprised in the samples or from which the samples are derived.
By applying this embodiment of the method of the invention, it is possible to find correlations between the difference in the phenotypic and/or genotypic state and changes in the metabolite profile for instance by performing metabolite co-response analyses.
The term "phenotypic state" refers to differences in the phenotype of the cell under investigation or the organism in which it resides. "Phenotype" means any kind of feature that can be detected and which is not a feature of the genome. Such phenotypic states may for example be visually identifiable such as a morphological or anatomical difference like they can be observed at different developmental stages. Phenotypic states may likewise manifest themselves by the composition of chemical compounds or the occurrence of a disease. Thus, the phenotypic states may for instance be a healthy state in comparison to one or more pathogenic states, different stages of a pathogenicity or an uninfected versus one or more infected organisms.
The term "genotypic state" reflects differences in the genome of the cells under investigation. Thus, if the samples are taken from different genotypic states of a cell, the term "cell" specifically refers to cells according to the definition given above which belong to the same taxonomic unit, but which differ in at least one genetic trait. Specifically, the "taxonomic unit" is a genus, preferably a species, and more preferably an even lower taxonomic rank such as a race, variety, cultivar, strain, isolate, population or the like. Most preferably, the taxonomic rank is an isogenic line with variance in only a limited number, preferably three, more preferably two genetic traits and most preferably one genetic trait, whereby "genetic trait" refers to a chromosomal region, a gene locus or, as it is preferred, to a gene. Typically, differences in the genotypic state can be differences between a wild-type organism and one or more corresponding mutant or transgenic organisms or between different mutant or transgenic organisms. A certain genotypic state may be stable or transient as is the case with transduced or transfected cells, for instance containing a plasmid, phage or viral vector. Advantageously, organisms of different genotypic state are analyzed when they are in the same developmental stage.

It is immediately clear that the terms "phenotypic" and "genotypic" states may overlap. In particular, normally a genotypic state, if the differing genetic trait(s) is/are expressed in the organism, lead(s) to a difference in the phenotype.

According to the above explanations, in a preferred embodiment of the method of the invention, the different phenotypic and/or genotypic states are different developmental stages, environments, nutritional supplies, taxonomic units, wild-type and mutant or transgenic genomes, infected and uninfected states, diseased and healthy states or different stages of a pathogenicity.

In a further preferred embodiment of the method of the invention as described hereinabove, said analysing further involves suitable statistical evaluation and correlation analyses of the data obtained and, optionally, network analyses.
This refers to any mathematical analyses method that is suited to further process the quantitative data provided by the method of the invention. This data represents the amount of the analyzed metabolites present in each sample either in absolute terms (e.g. weight or moles per weight sample) or in relative terms (i.e. normalized to a certain reference quantity).
Quantitative analyses involves suitable statistical evaluation and correlation analyses. The former includes normalization to the total content of the respective compounds, correction of background levels and the combination of the data sets obtained from different experiments (if more than one sample is analysed) into a single data sheet. Corresponding mathematical methods and computer programs are known to the skilled practitioner. Examples include SAS, SPSS and systatR. As the next step, the statistically pre-treated data may be subjected to a pairwise correlation analyses. Here series of pairs of data points from the analyzed compounds are looked at for correlation, whether positive or negative, for instance using Pearson's correlation coefficient.
In a preferred embodiment, the quantitative analyses referred to in the method of the invention furthermore involves network analyses. Network analyses aims at finding out higher order interplays of multiple factors on the basis of pairwise correlation data. If, according to one of the above-described preferred embodiments, metabolites and transcripts and/or proteins are quantitatively determined, for the obtained several

data sets, preferably each obtained from one sample, correlations between metabolites and proteins and/or transcripts as well as within these classes of compounds can be analyzed in order to derive information about the network regulation of biological systems, e.g. upon genetic or environmental perturbation. A comprehensive overview of methods for quantitatively analyzing data obtained according to the method of the invention including principle component analyses, "snapshot analyses", Pearson correlation analyses, mutual information and network analyses can be found in Fiehn (2001).

In a further aspect, the present invention relates to a set of isotopically labeled metabolites obtainable from a sample which comprises or is derived from a cell which has been maintained under conditions allowing the uptake of an isotopically labeled metabolizable compound so that the metabolites in said cell are saturated with the isotope with which said metabolizable compound is labeled.
The present invention also relates to such cells which can be cells as described above in connection with the method of the invention.
As is explained hereinbefore, the Isotopically labeled metabolites obtained from a biological sample in accordance with the method of the present invention may be used as a quantitative standard for the quantitative determination of the metabolites of a second biological sample. Thus, a set of these labeled metabolites is also an object of the present invention. Preferably, this set can be used to standardize results of a metabolome analyses conducted with the same species of cells as that from which the set of metabolites is obtained. However, it is also feasible that this set may be of use to standardize metabolite data obtained from a different species. This would generally require that metabolites of the set are identical with metabolites of the second biological sample. Identity can be determined or confirmed by using methods known in the art and described herein. For instance, the in vivo isotopically labeled metabolites obtained from yeast may be used as a quantitative standard for metabolites of plant cells since, for a considerable subset of each of these metabolites, the metabolites overlap such as the metabolites of the primary metabolic pathways.
As a further use of the set of isotopically labeled metabolites of the invention, or corresponding cells containing them, it is envisaged that the set or the cells can be

used as a qualitative standard in order to identify metabolites from a second, unlabeled biological sample.
The set of metabolites may be prepared in accordance with the above explanations for carrying out the method of the invention. For the purposes of storing and transporting that set, corresponding methods may be applied which are suitable in order to ensure that degradation of each kind of metabolite contained therein is at least minimized to a tolerable degree and which are known to a person skilled in the art.

In a further embodiment, the present invention refers to the use of the set of isotopically labeled metabolites mentioned above as a quantitative standard for determining the amount of one or more metabolites in a biological sample.

Furthermore, the present invention relates to a kit comprising an isotopically labeled metabolizable compound and a manual for use in carrying in out the method of the invention or the set of isotopically labeled metabolites described above.
The components of the kit of the invention may be packaged in containers such as vials in a storable and transportable form. If appropriate, one or more of said components may be packaged in one and the same container.

Additionally, the present invention relates to the use of an isotopically labeled compound that can be metabolized by a cell for labeling the metabolites in said cell in a saturating manner.
Such uses may be carried out in accordance with the above-outlined explanations for the method of the invention.

The present invention also relates to the use of an isotopically labeled compound that can be metabolized by a cell for the quantitative determination of metabolites in a biological sample comprising or being derived from said cell.
Such uses may be carried out in accordance with the above-outlined explanations for the method of the invention.

Likewise, the present invention relates to the use of an isotopically labeled compound that can be metabolized by a cell for analysing the metabolite profile of a biological sample comprising or being derived from said cell.
Such uses may be carried out in accordance with the above-outlined explanations for the method of the invention.

These and other embodiments are disclosed and encompassed by the description and examples of the present invention. All of the publications, patents and patent applications referred to in the specification in order to illustrate the invention are hereby incorporated by the reference in their entirety. Further literature concerning any one of the methods, uses and compounds to be employed in accordance with the present invention may be retrieved from public libraries, using for example electronic devices. For example the public database "Medline" may be utilized which is available on the Internet, for example under http://www.ncbi.nlm.nih.gov/PubMed/medline.html. Further databases and addresses, such as http://www.ncbi.nlm.nih.gov/, http://www.infobiogen.fr/, http://www.fmi.ch/biology/research_tools.html, http://www.tigr.org/, are known to the person skilled in the art and can also be obtained using, e.g., http://www.google.de. An overview of patent information in biotechnology and a survey of relevant sources of patent information useful for retrospective searching and for current awareness is given in Berks, TIBTECH 12 (1994), 352-364.
Furthermore, the term "and/or" when occurring herein includes the meaning of "and", "or" and "all or any other combination of the elements connected by said term".

The present invention is further described by reference to the following non-limiting figures, tables and examples.

<u>The Figures and the Tables show:</u>

Figure 1 shows the results of head-to-tail analyses of electron impact ionisation mass spectra of yeast metabolites extracted from GC-MS metabolite profiles.

The yeast metabolites succinic acid, glycine and glutamic acid were trimethysilylated prior to GC analyses. The number of silylated functional groups and the magnification factor of the high molecular mass range is indicated. Head-to-tail mass spectra are from separate GC-MS analyses of ambient $\delta^{13}C$- and ^{13}C-saturated yeast extracts. Insets to the right show the M^+ and $[M-15]^+$ fragment ranges of combined ^{13}C-isotopomer ratio (ITR) metabolite profiles. The isotopomer $[M-15]^+$ fragment pairs of succinic acid (2TMS), glycine (3TMS), and glutamic acid (3TMS) are M/Z 247_251, M/Z 276_278, and M/Z 348_353. Glutamic acid (3TMS) exhibited abundant molecular ions, M^+, M/Z 363_368.

Figure 2 depicts a comparison of ITR metabolite profiling (A, C) and conventional metabolite profiling (B,D).

Selected ion responses of ^{12}C- and ^{13}C-isotopomer fragment pairs, which represent the same substance from ambient $\delta^{13}C$- and ^{13}C-saturated yeast extracts (A, B), and fragments which represent the same isotopomer in two different experiments (Exp1 and Exp2) from either the ambient $\delta^{13}C$- or ^{13}C-saturated yeast culture (C, D) are plotted. ITR was performed in two GC-MS analyses (06, 10), whereas four GC-MS analyses were required for conventional metabolite profiling (ambient $\delta^{13}C$: 04, 08; ^{13}C-saturated: 05, 09). Pearson's linear correlation coefficients (r) and average coefficients of variation (cf) are shown in the insets.

Figure 3 represents a GC-TOF-MS metabolite profile of yeast strain BY4741.

Ticks below the total ion current trace of the main profile indicate the automated deconvolution of mass spectral components with S/N ≥ 100 which were performed by Pegasus chromatography data processing software. The inset shows selected ion traces of deconvoluted components from the shaded area of the main profile. **A** isoleucine (2TMS), M/Z = 158; **B** threonine (2TMS), M/Z = 117; **C** proline (2TMS),

M/Z = 142; **D** glycine (3TMS), M/Z = 174; **E** 2,2,3,3-d4-succinic acid (2TMS), M/Z = 251; **F** succinic acid (2TMS); M/Z = 247 (factor of magnification 10). The presence of 2,2,3,3-d4-succinic acid resulted from standard addition of a deuterated isotopomer.

Figure 4 depicts a clustering tree of identified, and non-identified MSTs from extracts of Saccharomyces cerevisiae strain BY4741 and pure standard compounds. MSTs were classified into groups by hierachical clustering of a complete symmetric matrix of pair-wise mass spectral match values (Table 4). 18 groups of MSTs were classified at a cut-off at approximately 50 % diversity (the MST groups are described in Example 6).

Figure 5 shows the results of a principal component analyses based on GC-TOF-MS metabolite profiles of extracts from a single batch culture of Saccharomyces cerevisiae strain BY4741 (A_{595} ~ 1.8). Four sampling strategies (n = 16) were employed, namely quenching into cold methanol (MEOH), collection onto filter disc (FILTER), collection by centrifugation without media wash (SPIN), and collection by repeated wash and centrifugation cycles (SPINW). Washes were performed with glucose-free SD medium. Principal components 1, 2, and 3 covered 57.4 %, 24.2 %, and 6.4 % of the total variance of the profile data set. Metabolite responses were normalised to the average metabolite response observed within each sample. Average relative standard deviation (RSD) of each of the sampling procedures is indicated. Underlying metabolite profiles, metabolite responses and relative standard deviations of all metabolites are presented in Table 6.

Figure 6 provides the results of a comparison of four co-response measures applied to metabolite profiles of Saccharomyces cerevisiae strain BY4741 (A_{595} ~ 1.8). Kendall's correlation coefficient is compared to Euclidian distance (A), mutual information (B) and Pearson's correlation coefficient (C). Each tuple represents a metabolite/metabolite co-

response. Arrows indicate position of exemplary bi-plots presented in double-log10 scale to the right. Four sampling strategies (n = 16) were employed, namely MEOH, FILTER, SPIN, and SPINW. The sampling techniques were as described within the legend to Figure 5. A complete overview of all pair-wise metabolite/metabolite co-response measures is given in Table 7.

Figure 7 shows metabolite bi-plots in double-log10 scale representing co-response behaviour of intermediates and a product of the tricarboxylic acid cycle. Oxaloacetic acid was below limits of detection in GC-TOF-MS profiles of yeast. **A**, malic acid/ aspartic acid; **B**, malic acid/ citric acid; **C**, fumaric acid/ malic acid; **D**, succinic acid/ fumaric acid. The sampling techniques are as described within the legend to Figure 5.

Figure 8 shows the common nearest and most distant neighbours of succinic acid, fumaric acid, and malic acid, as described by Kendall´s correlation coefficient. Values of correlation coefficients were coded by line style, ≥ 0.6 full line and ≤ -0.5 dotted line.

Figure 9 shows a continuous positive-ion MALDI-TOF-MS spectrum of an ambient δ^{13}C-yeast extract with 2,5-dihydroxybenzoic acid as matrix set to the expected mass range of NAD^+ (NADH) adducts, namely protonated molecular ions at m/z 664.11 (666.13), and sodium adducts at m/z 686.09 (688.12), respectively. The inset (^{12}C/^{13}C) shows a bar representation of the protonated molecular ion region from a ^{13}C-isotopomer ratio (^{13}C-ITR) MALDI-TOF-MS analyses. M/z 679.26 and 681.25 represent protonated NAD^+ and NADH, which were labeled with 15 ^{13}C-atoms. ^{13}C-saturated yeast extracts exclusively showed the labeled ions in the m/z 677 - 685 range (data not shown).

Figure 10 depicts a head-to-tail analyses of post source decay (PSD) fingerprints from separate MALDI-TOF-MS analyses of ambient δ^{13}C- (^{12}C PSD) and ^{13}C-saturated (^{13}C PSD) yeast extracts. Evident m/z differences of

parent ions and fragments were 15, 10, and 5 amu. The required mass window for the isolation of parent ions (~ ±3 amu) and subsequent PSD analyses did not allow separate monitoring of NAD^+ and NADH from mixtures.

<u>The following Examples illustrate the invention:</u>

Experimental set-up

<u>Strain information and in-vivo labeling</u>

Saccharomyces cerevisiae strains BY4741 (MATa; his3Δ1; leu2Δ0; met15Δ0; ura3Δ0) and BY4742 (MATα; his3Δ1; leu2Δ0; lys2Δ0; ura3Δ0) were obtained from the EUROFAN II worldwide gene deletion project (EUROSCARF collection, Frankfurt, Germany. http://www.uni-frankfurt.de/fb15/mikro/euroscarf/col_index.html) (Kelly, 2001; Winzeler, 1999). Strains were grown for 16-24 h in 25 - 250 ml liquid batch cultures on synthetic defined (SD) minimal medium with required auxotrophic supplementation and 20 g l^{-1} ambient δ^{13}C-glucose as major carbon source (Castrillo, 2003). For in-vivo ^{13}C-labeling ambient glucose was replaced by U-^{13}C-glucose (99 atom %, Isotech Inc., Miamisburg, USA). Auxotrophic and vitamin supplements were non-labeled.

For the control of residual SD medium components within cellular preparations from yeast cultures the media contained 4 g l^{-1} lactose (β-D-galactopyranosyl-(1,4)-D-glucose, Fluka, Buchs, Switzerland), which is not utilized by Saccharomyces cerevisiae.

<u>Cellular preparations from yeast cultures</u>

For all experiments 5 ml aliquots were taken from over-night yeast batch cultures grown to A_{595} ~ 1.8 . Sampling procedures were: (1) MEOH, quenching into –50°C cold methanol, subsequent centrifugation, and aspiration of supernatant (MEOH) (Castrillo, 2003; Gonzalez, 1997) with non-buffered quenching solution (see below);

(2) FILTER, vacuum collection onto 0.65 µm Durapore PVDF hydrophilic membrane filter discs (Millipore GmbH, Schwalbach, Germany); (3) SPIN, collection by gentle centrifugation and complete aspiration of supernatant without subsequent wash; (4) SPINW, collection by 2 repeated gentle centrifugation and wash cycles with carbohydrate-free SD media. All procedures were performed at 28°C if not mentioned otherwise. Cellular preparations were either immediately processed or shock frozen in liquid nitrogen. Routine sampling was MEOH, if not indicated otherwise. As monitored by the lactose-tracer molecule all sampling methods except SPINW contained low amounts of residual media components. Non-sample control experiments with fresh SD media and analyses of the initial cell free medium and at time of sampling were performed (data not shown)..

Preparation of intracellular yeast metabolites

Hot methanol/ chloroform extraction (15 min at 70°C), liquid phase partitioning into methanol/water (1:1, v/v), drying by vacuum centrifugation, and subsequent treatment with methoxyamine hydrochloride (MEOX) and N-methyl-N-(trimethylsilyl)-trifluoroacetamide (MSTFA) reagents for conventional yeast metabolite profiling of polar soluble material was down-scaled as described previously (Wagner, 2003). For the extended GC-TOF-MS analyses of yeast samples liquid partitioning by addition of water to the initial methanol/ chloroform extract was omitted. Instead the complete extract volume, ~ 700 µl, was dried by vacuum centrifugation.
Supplementation of quenching- or extraction-solution with recommended buffer systems (Castrillo, 2003; Gonzalez, 1997) for the preparation of intracellular yeast metabolites led to strong interferences of the buffer substances with either methoxyamination, silylation, or chromatographic performance of the final sample preparations. Therefore, buffering substances had to be avoided for GC-MS profiling.

^{13}C-isotopomer ratio (ITR) metabolite profiling

Extracts of intracellular yeast metabolites from ambient δ^{13}C- and ^{13}C-saturated cultures were combined in equal amounts prior to vacuum centrifugation. The ^{13}C-

saturated extract was treated as a stable isotope labeled, multiplex internal standard mixture. Each component of the resulting metabolite profiles was quantified by use of the respective ^{13}C-saturated compound. For this purpose ^{12}C/^{13}C response ratios of pre-selected isotopomer fragment pairs were calculated (Table 2). Specific isotopomer fragment pairs were assigned manually to each identified and non-identified metabolite using respective mass spectral entries from the collection of mass spectral metabolite tags (MSTs; see below). Prior to forming ratios responses of ^{13}C-saturated fragments were corrected for the contribution of naturally occurring ^{13}C-isotopomers to ambient δ^{13}C-preparations.

GC-MS technologies

Conventional GC-MS profiles were performed with a quadrupole type GC-MS system, namely a GC8000 gas chromatograph coupled to a Voyager mass spectrometer, which was operated by MassLab software (ThermoQuest, Manchester, UK). Modifications to the initial GC-MS profiling method (Fiehn, 2000a; Fiehn, 2000b) were, injection of 1 µl sample in splitless mode, use of a 5°C min^{-1} temperature ramp with final temperature set to 350°C on a 30 m x 0.25 mm inner diameter Rtx-5Sil MS capillary column with an integrated guard column (Restek GmbH, Bad Homburg, Germany), and use of alkane mixtures for the determination of retention time indices. These changes reflect recent optimisation which was performed with a GC-TOF-Pegasus II MS system (Leco, St. Joseph, USA). All GC-TOF-MS experiments were done on a Pegasus II TOF-MS system as detailed earlier for a diverse range of plant samples (Wagner, 2003)

MALDI-TOF-MS technologies

Yeast extracts were analysed by MALDI-TOF-MS (Voyager DE-PRO Biospectrometry Workstation, Applied Biosystems, Foster City, USA) set to positive ion detection in reflectron mode (Lerouxel, 2002). Settings for reflectron MALDI-TOF-MS and PSD were as recommended by the manufacturer. A 2,5-dihydroxybenzoic acid (10 mg ml^{-1}) matrix was mixed 1:1 (v/v) with polar fractions from yeast extracts

or pure compounds, which were dissolved in methanol: water (1:1, v/v). Slow crystallisation by air drying was essential for the laser desorption and ionisation of NAD^+ and NADH; microcrystalline samples exhibited complete signal suppression.

An exemplary study using the same MALDI-TOF-MS matrix previously demonstrated that stable isotope standardized MALDI-TOF-MS exhibited precise standard curves over two orders of magnitude and produced quantitative results in accordance with in-parallel gas chromatographic analyses (Kang, 2001).

Generation of a compendium MST library

MSTs (Table 3) were obtained through automated deconvolution of GC-TOF-MS chromatograms (ChromaTOF™ software, LECO, St. Joseph, USA). Mass spectra were collected into user libraries provided by NIST98 and AMDIS software (http://chemdata.nist.gov/mass-spc/Srch_v1.7/index.html and http://chemdata.nist.gov/mass-spc/amdis/; National Institute of Standards and Technology, Gaithersburg, USA) (Stein, 1999; Ausloos, 1999). MSTs were manually annotated and corrected for obvious errors caused by automated deconvolution. Mass spectra of low intensity and truncated or fused mass spectra which resulted from co-elution of compounds were rejected except for demonstrating of the presence of a labeled isotopomer.

Identification and classification of mass spectral metabolite tags (MSTs)

MSTs were identified by manually supervised standard addition experiments with pure commercially available substances. Required criteria for substance identification were chromatographic co-elution and high mass spectral similarity of MSTs observed within yeast samples to standard substances (Wagner, 2003) Co-elution and similarity were described by retention time index and mass spectral match values, respectively. Non-identified MSTs were tentatively analysed by best match with a customised MS library of standard substances and entries from the commercial NIST98 library (National Institute of Standards and Technology, Gaithersburg, USA). MSTs were classified by agglomerative hierarchical cluster analyses using Euclidian

distance measure and average linkage (Table 5, Figure 4). Cluster analyses was applied to a complete matrix of pair-wise mass spectral match values (Table 4) as described earlier (Wagner, 2003). Yeast MSTs and a selection of EI-TOF mass spectra from pure standard substances were co-classified.

Statistical analyses and visualisation of metabolite profiles

Principal component analyses (PCA), hierarchical clustering, calculation of Euclidian distance, Pearson's and Kendall's correlation coefficient, and mutual information was calculated using the S-Plus 2000 software package standard edition release 3 (Insightful, Berlin Germany), the programming language R version 1.6.1 and 1.6.2 (http://www.r-project.org) and the MetaGeneAlyse version 1.3 world wide web resource (http://metagenealyse.mpimp-golm.mpg.de/) (Daub, 2003).
The model for metabolic network representation was as suggested (Jeong, 2000) and overlay of correlation coefficients in accordance with modularity analyses in metabolic networks (Ravasz, 2002). Network visualisation and layout was performed using the Pajek (Batagelj, 1998) algorithm package available at http://vlado.fmf.uni-lj.si/pub/networks/pajek/.

Calculation of metabolite profiles

Each metabolite was represented by a single response value (Table 6). Within GC-MS profiles single metabolites may be represented by multiple derivatives, which are detected by respective MSTs, and each MSTs may be represented by more than one specific fragment (refer to Table 2 and Figure 1). In these cases an additive composite metabolite response was calculated rather than selecting a single MST and corresponding fragment.
Metabolite response was normalised to the average signal intensity of all MSTs, which were observed within each single GC-MS chromatogram. This strategy of data normalisation was mandatory prior to comparison of sampling technologies and analyses of metabolite co-response, because sampling technologies had variable and different recoveries of viable cells from the same batch culture. For example,

each wash cycle of SPINW sampling successively reduced recovery of viable cells (data not shown). Attempts failed to identify a constitutive metabolite, which would allow to exactly monitor the number and size of viable yeast cells within each preparation.

Example 1: Determination of the extent of saturation by in vivo ^{13}C-labeling

In order to determine the completeness of in vivo ^{13}C-labeling (saturation), yeast cells (yeast strain BY 4741; Kelly, 2001; Winzeler, 1999) were fed with U-^{13}C-glucose as the only carbon source except for auxotrophic and vitamin supplements, i.e. biotin, pantothenate, folic acid, inositol, niacin, p-aminobenzoic acid, pyridoxine, riboflavin, thiamine, bacto-yeast nitrogen base without amino acids, histidine, leucine, methionine, uracil, and inorganic salts, i.e. ammonium sulfate, boric acid, copper sulfate, potassium iodide, ferric chloride, manganese sulfate, sodium molybdate, zinc sulfate, potassium phosphate, magnesium sulfate, sodium chloride, calcium chloride that were non-labeled and extracts from these yeast cells were examined by conventional electron impact GC-MS for the content of different metabolites. As judged by the resulting mass spectra profiles, the majority of the detectable metabolites from the yeast cells was completely labeled. In detail, ambient (i.e. naturally occurring) $^{12}C/^{13}C$-carbon ($\delta^{13}C$-) isotopomer composition was found for uracil, methionine, histidine, nicotinic acid and inositol in extracts prepared from cultures supplemented with U-^{13}C glucose. Non-labeled leucine and panthothenic acid were frequently observed, however these metabolites were only abundant at levels close to detection limits. Other vitamins comprised by SD media, e.g. biotin, folic acid, p-aminobenzoic acid, pyridoxine, riboflavin, and thiamine, were below limits of detection or not accessible by GC-MS technology.

Furthermore, homocysteine, and inositol-phosphate were detected devoid of ^{13}C-label. A still non-identified conjugate of inositol exhibiting high similarity to galactinol was partially labeled, and uridine carried 5 out of 9 possible ^{13}C atoms. These findings indicate: (1) synthesis of homocysteine from methionine by 5-methyltetrahydropteroyltri-L-glutamate:L-homocysteine S-methyltransferase (EC 2.1.1.14; MET6), (2) a pathway from inositol to inositol-phosphate possibly through

phosphatidylinositol synthase (2.7.8.11; PIS) and phospholipase C (3.1.4.11; PLC1) activity, and (3) uracil scavenged by uracil phosphoribosyltransferase (EC 2.4.2.9; FUR1) and subsequent phosphatase action.

Example 2: "Inverse labeling" of yeast cells

L-lysine supplementation of yeast strain BY 4741 was tested in ^{13}C-saturated cultures. Lysine is the complementary auxotrophic marker substance of the second Saccharomyces cerevisiae strain BY4742 used by the EUROFAN II worldwide gene deletion project (Kelly, 2001; Winzeler, 1999). ^{13}C-labeling of lysine was suppressed in strain BY4741 when supplemented with this amino acid. Moreover, 2-aminoadipic acid accumulated only in strain BY4742. This results indicates that the bi-directional L-lysine synthesis and degradation pathway which comprises the activities of L-aminoadipate-semialdehyde dehydrogenase (EC 1.2.1.31; LSY2, LYS5), NADP$^+$-, L-glutamate-forming saccharopine dehydrogenase (EC 1.5.1.10; LYS9), and NAD$^+$-, L-lysine-forming saccharopine dehydrogenase (EC 1.5.1.7; LYS1) is interrupted.

Example 3: Identification of ^{12}C- and ^{13}C-isotopomer pairs

Reliable identification of pairs of ^{12}C- and ^{13}C-isotopomers which represent the same metabolite is a prerequisite for accurate isotopomers ratio (ITR) metabolite profiles. Pairs of isotopomers may be identified based on mass spectral fragmentation as well as by chromatographic retention. Initial GC-MS experiments demonstrated that derivatives of commercially available deuterated compounds had significantly smaller retention time indices (RI) than non-deuterated compounds. For example, 2,3,3,3-D4 alanine (2 TMS), 2,3,3-D3-aspartic acid (3 TMS), 2,3,3,3-D4 alanine (3 TMS), 2,2,3,3-D4-succinic acid (2 TMS), and 2,3,4,4,4,5,5,5-D8- valine (2 TMS) eluted 1.1, 1.8, 2.3, 2.5, and 3.8 RI units prior to respective non-deuterated isotopomers.
In contrast, commercially available ^{13}C-labeled compounds exhibited only minor shifts in RI. This observation was confirmed by a selection of 66 ^{13}C-labeled mass spectral metabolite tags (MSTs) observed in standard GC-MS profiles. This testing set of MSTs was selected according to high mass spectral peak purity and presence

of at least one abundant and specific fragment which could be employed for selective ion quantification and RI monitoring. The selection comprised derivatives of amino acids, organic acids, sugars, sugar alcohols, sugar phosphates, and a set of 34 non-identified MSTs. The complete list including all available and manually evaluated GC-EI-MS isotopomer fragment pairs is listed in Table 2 (see infra). RI of ^{13}C-labeled compounds was on average only 0.28 (± 0.53 SD) units smaller than those of non-labeled compounds. This slight shift of RI was equivalent to approximately 0.3 sec of retention time.

Interpretation of the EI-MS fragmentation pattern of pairs of ambient $\delta^{13}C$- and ^{13}C-isotopomers allowed the verification of metabolite identity. Typical EI mass spectra of succinic acid (2 TMS), glycine (3 TMS), and glutamic acid (3TMS), are shown in Figure 1. The head to tail analyses of ambient $\delta^{13}C$- and ^{13}C-EI-mass spectra allowed an easy identification of isotopomer fragment pairs for use in ITR metabolic profiling. For example, glutamic acid ($C_5H_9NO_4$) forms a TMS derivative with the sum formula $C_{14}H_{33}NO_4Si_3$ and a relative molecular mass of 363. The molecular ion M^+, m/z 363, and the $[M-15]^+$ fragment, m/z 348, which is generated by typical neutral loss of a CH_3-radical from a TMS group, correspond to ions being characterized by m/z 368 and m/z 353 in which all 5 carbon atoms of glutamic acid are ^{13}C-labeled. The fragment $[M-117]^+$, m/z 246, can be matched with the corresponding ^{13}C-isotopomer fragment, m/z 250. These fragments are formed by neutral loss of a trimethylsilylated carboxyl group, which contains one of the 5 carbon atoms of the glutamic acid. The M^+ and $[M-15]^+$ fragments of ambient $\delta^{13}C$- and ^{13}C-saturated succinic acid (2 TMS), glycine (3 TMS) and glutamic acid (3TMS) are shown in the insets of Figure 1. These mixed mass spectra were obtained from ^{13}C-ITR metabolite profiles, i.e. combined analyses of ambient $\delta^{13}C$- and ^{13}C-saturated yeast extracts within single chromatograms. The chosen examples also demonstrate the necessity to correct ^{13}C-ITR metabolite profiles for ambient ^{13}C-isotopomer abundance, especially when the available mass spectral fragments for ^{13}C-ITR metabolite profiles contain only 1 or 2 labeled carbon atoms.

<u>Example 4:</u> Comparison of ^{13}C-ITR metabolite profiles with conventionally produced metabolite profiles

^{13}C-ITR metabolite profiles produced by combining equal amounts of ambient δ^{13}C- and ^{13}C-saturated yeast extracts into one GC-MS analyses were compared with conventional, i.e. separate, GC-MS profiles of the same extracts. The above-mentioned testing set of yeast MSTs was used for this comparison. Each MST was quantified by up to 3 manually validated isotopomer fragment pairs Table 2 (see infra). This experiment was performed with the aim to establish whether ITR metabolite profiling which utilizes internal standardisation by each the ^{13}C-labeled compounds is equivalent with conventional metabolite profiling. The latter approach was shown previously to operate successfully by external quantification (Fiehn, 2000a; Roessner, 2000).

Two yeast cultures were grown from the same colony in liquid SD medium. One culture was supplemented with ambient δ^{13}C-glucose, the second with U-^{13}C-glucose. Extracts of these cultures were either analysed separately or combined for ^{13}C-ITR before derivatisation. An initial experiment (Exp1) was repeated by taking a second sample from the same culture after a 15 min time interval (Exp2).

Two comparisons were performed based on the resulting metabolite profiles. (1) Comparison of Exp1 with Exp2 demonstrated the analytical variability, by means of re-analysing the same cultures (Figures 2C and 2D). (2) Comparison of the GC-MS responses of the labeled and non-labeled isotopomer fragment pairs showed the effect of ^{13}C-saturation on metabolic profiles (Figures 2A and 2B). Both comparisons were done either by ITR metabolite profiling (Figures 2A and 2C; ITR GC-MS analyses 06 and 10) or by conventional metabolite profiling (Figures 2B and 2D; ambient δ^{13}C GC-MS analyses 04 and 08; ^{13}C-saturated GC-MS analyses 05 and 09). GC-MS analyses 04, 05 and 06 represented Exp1, while analyses 08, 09, and 10 comprised Exp2. Pearson's linear correlation coefficient applied to the comparison of the experiments as well as to the influence of ^{13}C-saturation on the metabolic profiles demonstrated equivalence of ITR metabolite profiling and conventional metabolite profiling (Figure 2, inset).

The average coefficient of variation was determined by using all fragment pairs which contributed to each of the comparisons. Again results of ITR metabolite profiling and conventional metabolite profiling were equivalent, however, average coefficients of correlation were smaller in ITR metabolite profiling analyses (Figure 2, inset).

Most of the labeled isotopomers from the ^{13}C-saturated culture were present in amounts almost equal to the ^{12}C-isotopomers from the ambient $\delta^{13}C$-culture. The average $^{12}C/^{13}C$-isotopomer ratio of all pairs from the complete MST testing set was 0.79 (± 0.40 SD). However, some substances exhibited extreme differences, the ratios ranging between 0.01 and 2.98. These observations indicated that the process of ^{13}C-saturation alone may alter the levels of metabolites. Therefore, ITR metabolite profiling analyses of multiple samples should be standardised by extracts from a single large ^{13}C-saturated culture and corrected for the systematic error of ^{13}C-labeling.

<u>Example 5:</u> Preparation of a compendium of MSTs

Compilations of MSTs from biological samples represent an approach analogous to sequencing projects of expressed sequence tags (EST). We characterised the relevant major metabolites of yeast samples, obtained mass spectra and retention time indices for reliable metabolite identification, and finally generated means for metabolite-specific relative quantification.

Recently introduced GC-TOF-MS technology (van Deursen, 2000; Wagner, 2003) was adapted to the metabolic profiling of yeast. Fast scanning GC-TOF-MS systems are ideally suited for metabolite compendium projects. These systems allow automated and comprehensive deconvolution of mass spectral components from highly complex samples without user intervention. Moreover, this novel technology combines the advantages of high chromatographic resolution and reproducibility with the equally high reproducibility and acquisition rate of non-scanning time-of-flight MS-technology. In vivo stable isotope labeling was used to facilitate one of the most time-consuming steps in establishing metabolite profiling of any given biological sample type, i.e. the task to differentiate between MSTs which originate from yeast metabolizm and MSTs which represent experimental contaminations. The stable isotope label was introduced as a chemically defined and predominant carbon source and was used to detect all metabolic conversions originating from this carbon source. The apparent complexity of initial metabolic profiles of polar extracts from yeast was lower than profiles generated for instance from plant sources. We increased the final

efficiency of multi-parallel GC-TOF-MS analyses by adapting metabolic profiling to combined chloroform and methanol extracts from yeast which contained lipid metabolites in addition to the metabolites obtained by polar extraction as described earlier. Further attempts to increase the amount of yeast extract to be applied to GC-TOF-MS analyses in order to maximise the number of simultaneously monitored compounds were limited by matrix effects, which were brought about by four predominant compounds, phosphoric acid (3TMS), glycerol (3TMS), glucose (MX, 5TMS), and trehalose (8TMS). The matrix effects resulted (1) from excess phosphoric acid within extracts, which reduced the silylation strength of the MSTFA reagent and (2) from chromatographic overload of derivatives which produced peak deformation artefacts in the vicinity of major peaks. The final amount of yeast extract was adjusted to avoid these matrix effects (Figure 3). Thus the efficiency of multi-parallel GC-TOF-MS analyses was increased, for the time being without introducing time-consuming pre-fractionation and enrichment protocols.

A compendium of GC-TOF-MS metabolite tags was separately compiled from ambient $\delta^{13}C$- and ^{13}C-saturated yeast extracts from over-night batch cultures of Saccharomyces cerevisiae strain BY4741. In order to obtain different samples the metabolite profiles of which can be compared, different sampling protocols were applied, namely quenching into cold methanol (MEOH), collection onto filter disc (FILTER), collection by centrifugation without media wash (SPIN), and collection by repeated wash and centrifugation cycles (SPINW). The initial set of automatically retrieved mass spectra was manually curated to select MSTs of metabolic origin. The criteria applied for curation were: repeated occurrence of the mass spectral component ($n > 3$), reproducible fragment composition, signal to noise ≥ 50, and presence of a co-eluting ^{13}C-isotopomer. Mass spectra of metabolite derivatives devoid of carbon, and metabolite derivatives originating from ambient $\delta^{13}C$ auxotrophic and vitamin supplementation were included. The MST compendium is depicted in Table 3.

Example 6: Identification and classification of MSTs

For the identification of MSTs, mass spectral matching algorithms were employed, which are contained in publicly available mass spectral search and comparison software (Stein, 1999; Ausloos, 1999). The underlying procedures are analogous to those employed in BLAST analyses of ESTs. MSTs were compared to commercial MS collections and a custom EI-TOF-MS library. Best matches were assigned for a preliminary identification (Table 3). However, the presence of multiple chemical isomers with close to identical mass spectral fragmentation patterns make it necessary to conduct standard addition experiments in order to obtain a precise identification. We sampled 180 MSTs (Table 3) and identified 78 tags which represented 67 yeast metabolites (Table 1). The range of identified compounds comprised amino acids, organic acids, sugars, polyols, purines and pyrimidines, phosphorylated compounds, fatty acids and sterols (Table 1).

A non-biased, automated classification of MSTs has previously been established (Wagner, 2003). This approach towards a non-biased mass spectral classification utilises the observation that two mass spectra of the same compound do not only match best but also have similar match values when compared to other, even highly different, mass spectra. This method of MST classification was applied to yeast MSTs and a framework of known mass spectra obtained from standard addition experiments. We inferred 19 groups of MSTs from agglomerative hierarchical clustering by average linkage of Euclidian distances and a cut-off at approximately 50 % diversity (Figure 4 and Table 5). The groups of MSTs comprised alkanes which were included for RI standardisation (group 1; 0/7 non-identified), di- and tri saccharides (group 2; 4/17 non-identified), hexose pyranosides (group 3; 8/9 non-identified), hexonic acids and inositol (group 4; 4/10 non-identified), aldohexose methoxyamines (group 5; 3/12 non-identified), a group of non-identified MSTs similar to polyols (group 6; 5/5 non-identified), ketohexose- and pentose methoxyamines (group 7; 0/14 non-identified), hexitols, pentitols and hexonolactones (group 8; 2/19 non-identified), a group of standard caffeoylquinic acids (group 9; 0/8 non-identified), organic acids and purine nucleosides (group 10; 8/34 non-identified), C3-C5 polyols, hydroxy acids and sugars (group 11; 9/30 non-identified), phosphates (group 12; 9/34 non-identified), amines and amino acids with primary amino-group (group 14; 8/26 non-identified), fatty acids and sterols (group 15; 7/15 non-identified), a standard set of phenylpropanoic acids (group 16; 0/9 non-identified), a heterogenous group of

mostly cyclic compounds comprising phenyl-, indoyl-, imidazol-, pyrimidine-, and purine-residues (group 17; 12/31 non-identified), and a group dominated by amino acids (group 18; 9/60 non-identified). Group 0 (17 MSTs) and group 3 (4 MSTs) represented mass spectra with unclear classification. Most of those mass spectra, which represented identical compounds were found to be either nearest neighbours or were classified to belong to the same branches of the clustering tree. The mass spectrum of leucine (2TMS) was entered in duplicate in order to monitor the position of a pair of identical mass spectra within the clustering tree (Figure 4). Some yeast MSTs of group 0, namely methionine (2TMS), adenine (2TMS), and proline (2TMS), did not sort as expected. This observation was caused by errors of automated deconvolution due to low abundance or due to co-elution of other MSTs. Clustering after substitution of the matrix by a minimum threshold match value allowed improved grouping of missorted mass spectra, but obscured classification of those MSTs without high similarity to other MSTs or standard MS. More elaborate, preferably supervised-learning algorithms applied to matrices of match values as well as directly to mass spectra and RI will lead to improved and more precise classification results and increased robustness of identification.

Example 7: Application of metabolite profiling analyses

Metabolites are embedded within a network of fast enzyme and transport reactions. Not unexpectedly, metabolite co-response was discovered within sets of GC-MS metabolite profiles from plant samples. This co-response was subsequently discussed to yield novel information about biochemical mechanisms of metabolite interactions. Because reaction rates of metabolic conversions are in general significantly higher than rates of protein or mRNA turn-over, this type of analyses highly depends on a quick quenching of the metabolizm during sample preparation. However, shock-freezing in liquid nitrogen, which was described earlier to be successful for plant samples, cannot be applied to yeast liquid cultures. For this reason, four other sampling regimes were assessed. These were applied to aliquots from a single batch culture. The sampling strategies were as described above (see Example 5), namely MEOH-, FILTER-, SPIN-, and SPINW-sampling by two repeated wash and centrifugation cycles of SD medium without carbohydrate source. The

metabolic perturbation induced by the respective sampling technologies was monitored by GC-TOF-MS metabolite profiles.

Principal component analyses (PCA) of all GC-TOF-MS metabolite profiles demonstrated that each of the sampling strategies exhibited specific metabolic characteristics (Figure 5). Sampling by repeated wash and centrifugation cycles (SPINW) with glucose-free SD medium was distinct from SPIN sampling and other sampling methods as described by principal component 1, which comprised the bulk variance, 57.4 %, of this experiment. Component 2, which held 24.2 % of total variance, separated sampling by centrifugation, i.e. SPIN and SPINW, from other sampling technologies. Component 3 comprising 6.4 % of total variance still allowed separation of MEOH from FILTER samples. All subsequent principal components were of low descriptive value with respect to the effect of the four sampling technologies. Analyses of the first three component loadings showed that lysine, asparagine, leucine, homoserine, methionine, arabinose, glycerol, octadecanoic acid, and 15 non-identified MSTs contributed most to the variance introduced by the choice of experimental perturbation (Table 6).

All sampling methods tested had a similar range of reproducibility as was indicated by the average relative standard deviation (RSD) of all replicate metabolite measurements (Figure 5). However, reproducibility of metabolite measurements were in some cases much lower than observed in plant samples. For example, the most widely accepted method, i.e. sampling of yeast cultures into cold methanol (MEOH), exhibited high variation for aspartic and glutamic acid, 67.2 % and 91.6 % RSD, respectively. This high variance was not caused by a trend over time of sampling or GC-TOF-MS analyses. In contrast, we demonstrated that other sampling strategies allowed highly reproducible measurements of these compounds, as was indicated for example by 18.0 % RSD with aspartic acid after FILTER sampling and 7.0 % RSD with glutamic acid after SPINW sampling. A complete overview of detailed metabolite-specific data is given in Table 6.

The data provided herein point toward the conclusion that some metabolite pools were in fast transition during or in between MEOH sampling. With respect to some metabolites, for example aspartic acid (Figure 7A) and glutamic acid, fast SPIN sampling was highly similar to MEOH sampling in exhibiting rapidly changing

metabolite pools. Finally, slower sampling technologies, like FILTER and SPINW, apparently allowed adjustment of stable metabolite pools prior to sampling.

Example 8: Metabolite co-response analyses

The analyses presented in Example 7 appear to reflect rapidly changing pool sizes of some metabolites. Thus, the metabolic perturbations, which were caused by the sampling procedures, were employed in order to gain insight into metabolite/metabolite interactions. Four co-response measures, namely Pearson's correlation coefficient, Kendall's correlation coefficient, mutual information (Steuer, 2002), and Euclidian distance, were applied to characterise all pair wise metabolite combinations. The results of these analyses are shown in Table 7.
Pearson's correlation coefficient and Kendall's correlation coefficient were applied to screen for linear co-response, which was reported to prevail in similar analyses of plants. The combination of both parametric and non-parametric tests allowed a preliminary evaluation of the import of outlying measurements on each metabolite co-response. Only a small fraction of apparent linear metabolite co-responses were caused by outlying metabolite measurements (Figure 6C). When comparing Kendall's and Pearson's correlation coefficients, which were applied to the same metabolite pairs, we observed a roughly sigmoidal relationship with positive and negative linear correlation distributed almost equally. A typical example of a negative linear co-response referring to the metabolite pair glycine/uracil is shown in Figure 6C.
Mutual information of metabolite pairs plotted over Kendall's correlation coefficient shows a minimum at Kendall's correlation coefficient close to zero. The mutual information measure confirmed positive and negative linear co-response. Moreover, selecting metabolite pairs with high mutual information and low Kendall's correlation coefficient allowed to discriminate non-linear or, as shown for glycine and alanine (Figure 6B), conditionally linear metabolite co-response.
Euclidian distance proved to be a measure apparently independent of linear correlation (Figure 6A) or mutual information (data not shown). Euclidian distance, however, was highly efficient in selecting metabolite co-responses which exhibited low variance of both metabolites.

Because each of the correlation measures had different properties, it was refrained in the present work from global hypothesis-free metabolite classification through cluster analyses based on any single distance measure. Instead by selecting intermediates and products of the tricarboxylic acid cycle, we posed the question as to whether the metabolites of a common pathway may be correlated. Succinic acid, fumaric acid, malic acid, aspartic acid, and citric acid were covered by the GC-TOF-MS analyses of yeast cultures presented herein. Aconitic acid, isocitric acid, and 2-oxoglutaric acid can be analysed by GC-TOF-MS profiling but were below limits of detection in this experiment. In a first approach, we focused on those metabolite co-responses which refer to direct links by biochemical reactions (Figure 7). Highly linear correlations were observed for succinic acid, fumaric acid and malic acid, which were maintained throughout all types of sampling (Figures 7C and 7D). By contrast, malic acid and citric acid or aspartic acid, respectively, adopted seemingly independent sampling specific states (Figures 7A and 7B). These states were either linear (Figures 7A and 7B; FILTER subset) or of highly variable and non-linear nature. Other metabolites, which are known to be directly interlinked by biochemical reactions, were also found to be correlated, for example lanosta-8,24-dien-3-beta-ol and ergosterol, glucose-6-phosphate and fructose-6-phosphate, or hexadecanoic acid and octadecanoic acid (Table 7).

In addition, interactions which did not follow classical pathway definitions were found within the data set of metabolite co-responses. For example, we selected a group of corresponding metabolites from a biochemical path of interest, namely succinic acid, fumaric acid, and malic acid, and searched for common closest neighbours. The 3 closest neighbours of this group of organic acids were glyceric acid and two non-identified metabolites as judged by positive Kendall's correlation coefficient. In addition lysine, glycine, and glutamic acid were most distant as judged by negative Kendall's correlation coefficient. An overview of this analyses is shown as a network representation (Figure 8).

<u>Example 9:</u> ^{13}C-ITR metabolite profiling by MALDI-TOF mass spectrometry

Metabolite profiling by GC-TOF-MS was shown to cover about 11% of the 584 yeast metabolites which were predicted by genome-scale reconstruction (Forster, 2003). However, this approach is mainly restricted by the limited scope of the GC-TOF-MS technology. The focus on specific classes of compounds with common properties is inherent to this as well as to any other analytical technology. For this reason, it is demonstrated in connection with the present invention that metabolite profiling using ^{13}C-in vivo labeling can be extended to MALDI-TOF-MS. MALDI-TOF-MS represents a mass spectral technology, which (1) cannot rely on chromatography for the confirmation of substance identity, (2) is highly sensitive to matrix suppression effects during laser desorption and ionisation, and (3) is not suited for external quantitative calibration. However, using MALDI-TOF for quantification with internal standard substances which are labeled by stable isotopes is an accepted procedure in connection with metabolite flux analyses (Wittmann, 2002; Wittmann, 2001). By nicotinamide adenine dinucleotide (NADH; $C_{21}H_{29}N_7O_{14}P_2$), an ubiquitous metabolic co-factor was chosen which allowed the demonstration of prerequisites essential to the ^{13}C-ITR approach.

Yeast extracts were treated as described above (see Example 4) to yield samples of a third experiment (Exp3). These samples were each harvested from the same batch cultures. Extracts with ambient $\delta^{13}C$ composition, extracts with ^{13}C-saturated metabolites, and an equal mixture of both extracts were analysed. Screening of MALDI-TOF spectra from the ambient $\delta^{13}C$ extract revealed protonated molecular ions of NAD^+ and NADH at m/z 664.11 and m/z 666.13, as well as sodium adducts at m/z 686.09 and 688.12 (Figure 9). These identifications were supported by commercial preparations of NAD^+ and NADH. The mass resolution of the MALDI-TOF system did not allow separation of the mono-isotopic ^{12}C-NADH ion from the A+2 isotopomer of ambient NAD^+. Therefore, analogous to the quantification of glycine (3TMS) (Figure 1), correction will be required for the determination of NADH in the presence of NAD^+. In addition, MALDI-TOF generated a continuous evenly spaced background of signals (Figure 9).

Within the mixed sample (Figure 9, inset), we found isotopomers of the protonated molecular ions of NAD^+ and NADH, which contained 15 ^{13}C-atoms out of 21 carbon atoms present within NAD(H). Small amounts of labeled sodium adducts were present (data not shown). The presence of only 15 labeled carbon atoms was in

agreement with the incorporation of non-labeled nicotinamide moieties into NAD(H), which originated from the nicotinic acid vitamin supplement contained in the yeast SD medium. The presence of non-labeled nicotinic acid ($C_6H_5NO_2$) in ^{13}C-labeled yeast extracts was demonstrated above (Example 1).

The identification of NAD(H) within yeast extracts was confirmed by post source decay (PSD) fingerprints of the protonated molecular ion cluster which were recorded separately from the ambient $\delta^{13}C$ and the ^{13}C-saturated yeast extracts (Figure 10). Analogous to the comparison of GC-EI-MS fragmentation pattern of isotopomers (Figure 1), head-to-tail analyses of PSD fingerprints allows the verification of the correct choice of isotopomer pairs. Moreover, fragment analyses of the ^{12}C-PSD and the ^{13}C-PSD revealed the successive loss of three moieties containing 5 carbon atoms each, namely two ribose units and one adenine building block, as was indicated by mass differences of 5, 10, and 15, respectively. Due to the restricted resolution of PSD analyses, separate fingerprints of the protonated ions of NAD^+ and NADH could not be obtained from mixtures. However, commercially available preparations of NAD^+ and NADH indicated that some PSD fragments, for example the fragment m/z 649.4 $[M-17]^+$, were highly specific. Fragment m/z 649.4 may result from facilitated neutral loss of NH_3 from the protonated NADH molecular ion. MALDI-TOF preparations of commercially available NAD^+ exhibited variable amounts of NADH mainly in the form of ion m/z 666.13, whereas NAD^+ was not detectable in preparations from NADH. This last finding indicated that the chosen MALDI-TOF procedure generates a reducing environment for chemical analyses which requires monitoring.

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Table 1

Table of yeast metabolites, which were represented by at least one mass spectral tag (MST). Identification of MSTs was performed by standard addition experiments. Identification required co-elution, mass spectral similarity, and presence of differentially labeled isotopomers.

Amino acids
2-Aminoadipic acid
Alanine
Arginine
Asparagine
Aspartic acid
Cysteine
Glutamic acid
Glutamine
Glycine
Histidine
Homocysteine
Homoserine
Isoleucine
Leucine
Lysine
Methionine
Ornithine
Phenylalanine
Proline
Pyroglutamic acid
Serine
Threonine
Tryptophan
Tyrosine
Valine

Organic acids
Citramalic acid
Citric acid
Erythronic acid
Fumaric acid
Gluconic acid
Glyceric acid
Malic acid
Pantothenic acid
Succinic acid

Miscellaneous
Adenine
Ethanolamine
Nicotinic acid
Uracil
Urea

Fatty acids
9-(Z)-Octadecenoic acid
Hexadecanoic acid
Octadecanoic acid
Octadecenoic acid

Sterols
Ergosterol
Lanosta-8,24-dien-3-beta-ol

Sugars
alpha-D-Methylglucopyranoside
Arabinose
Ribose
Fructose
Fucose
Glucose
Isomaltose
Mannose
Trehalose

Polyols
Erythritol
Glycerol
myo-Inositol
Mannitol
Ribitol
Sorbitol

Phosphates
Fructose-6-phosphate
Glucose-6-phosphate
Galactose-6-phosphate
Glyceric acid-3-phosphate
Glycerol-2-phosphate
Glycerol-3-phosphate
Phosphoric acid

Table 2

The table includes all manually evaluated GC-EI-MS isotopomer fragment pairs of identified and non-identified metabolite derivatives used for ^{13}C-ITR metabolite profiling. The table comprises names of metabolite derivatives or of best matches, mass spectrum identifier (MS-ID) for cross-referencing with Table 3, mass to charge ratio (M/Z) characterising the fragment isotopomer pairs and deviation of retention time indices (ΔRI).

Table 3

Datafile in the format *..msp[a] containing all curated GC-EI-TOF-MS mass spectra of MSTs from extracts of Saccharomyces cerevisiae strain BY4741.

The spectrum name was designed to allow sorting according to isotopomer, retention time index, experiment, and name, for example 12C_1625.9_1274EC17_Glutamic acid (3TMS) or 12C_1802.0_1313EC75_[706; Xylitol (5TMS)]. Retention time indices are as observed within the indicated experiment. Names represent identifications by co-elution and mass spectral match[b]; names in brackets indicate non-identified compounds and include the best mass spectral match. The chemical ID field was used to group isotopomer mass spectra by a common mass spectral ID (MS-ID), for example 163001-10-1 and 163001-11-1 representing ambient $\delta^{13}C$- and ^{13}C-saturated isotopomers of glutamic acid (3TMS). This identifier does not represent a CAS registry number. The formatting of this field is predefined by AMDIS software.

[a] The file format *.msp can be imported into NIST98 and NIST02 mass spectral comparison software (to be downloaded from http://chemdata.nist.gov/mass-spc/Srch_v1.7/index.html or AMDIS software (to be downloaded from http://chemdata.nist.gov/mass-spc/amdis/).

[b] By-products observed in preparations of reference substances were marked (BP).

Table 4

Matrix of all mass spectral similarities of the MSTs from yeast which are presented in Table 3. A complete pair-wise matching was performed with NIST98 mass spectral search and comparison software.

Table 5

Table of identified and non-identified MSTs from extracts of Saccharomyces cerevisiae strain BY4741 and pure standard compounds. MSTs were classified into groups by hierarchical clustering of the complete symmetric matrix of pair-wise mass spectral match values (Table 4). The resulting clustering tree is shown in Figure 4.

Table 6

Table of metabolite responses from GC-TOF-MS metabolite profiles of four sampling strategies (n = 6), namely MEOH-, FILTER-, SPIN- and SPINW-sampling by two repeated wash and centrifugation cycles. All samplings were performed on a single batch culture of Saccharomyces cerevisiae strain BY4741 (A_{595} ~ 1.8). Metabolite responses were normalised by the average metabolite response observed within each sample. MSTs and fragments which comprised the metabolite responses in this set of experiments are indicated. Metabolites exhibiting more than 75% missing data in all types of sampling strategies were removed. Table 6A depicts the raw data values which gave rise to the average values depicted in Table 6B.

Table 7

Table of all pair-wise metabolite/metabolite co-response measures. Number of available pair-wise measurements, Euclidian distance, mutual information, Kendall´s- and Pearson´s correlation coefficient were calculated from the metabolite responses presented in Table 6. The global information content of the correlation measures is demonstrated in Fgure 6.

Table 2

DERIVATIVE [BEST MATCH; NAME]	MS-ID	ISOTOPOMER PAIR M/Z	Δ RI
Alanine (2TMS)	110001	116_118	0.00
		190_192	0.00
		218_221	0.18
Glycine (3TMS)	133001	174_175	0.00
		248_249	0.00
		276_278	0.36
Threonine (2TMS)	132001	117_119	0.57
		219_221	0.93
		130_133	-0.75
Alanine (3TMS)	138002	188_190	0.00
		100_102	0.00
		262_264	0.18
Serine (3TMS)	138001	204_206	0.30
Aspartic acid (3TMS)	152002	232_235	0.00
		292_294	0.00
		306_309	0.25
Pyroglutamic acid (2TMS)	153002	156_160	0.00
		230_234	0.23
		258_263	0.23
Glutamic acid (3TMS)	163001	246_250	0.23
		128_131	0.00
		230_234	0.23
Phenylalanine (2TMS)	164001	218_220	0.45
		192_200	0.45
		266_274	0.23
Asparagine (3TMS)	168001	116_118	0.00
Ornithine (3TMS)	176006	174_175	0.23
		348_353	0.00
Ornithine (4TMS)	182002	142_146	0.00
		174_175	0.23
		420_425	0.00
Arginine (5TMS)	183001	157_161	0.25
		256_261	0.20
		373_379	0.43
Tyrosine (2TMS)	189006	179_186	0.25
		91_98	0.71

Lysine (4TMS)	192003	156_161	1.67
		174_175	0.00
		317_322	0.27
Lysine (3TMS)	186002	174_175	0.00
		200_206	0.00
		258_264	0.00
Tyrosine (3TMS)	194002	218_220	0.58
		280_288	0.00
		354_362	0.00
Glycerol (3TMS)	129003	218_221	0.00
		263_265	0.20
		293_296	0.00
Fructose methoxyamine (5TMS)	187002	217_220	0.23
		307_310	0.45
Fructose methoxyamine {BP} (5TMS)	188004	307_310	0.96
		217_220	0.00
Mannose methoxyamine (5TMS)	188002	205_207	0.23
		217_220	0.00
		319_323	0.23
Glucose methoxyamine (5TMS)	189002	364_368	-0.06
		343_349	0.24
		291_294	0.00
Glucose methoxyamine {BP} (5TMS)	191001	364_368	1.12
		343_349	1.97
		291_294	1.39
Mannitol (6TMS)	193002	217_220	1.06
		319_323	0.00
Sorbitol (6TMS)	193001	217_220	0.00
		319_323	0.00
Trehalose (8TMS); alpha-D-Glc-(1,1)-alpha-D-Glc	274002	451_457	3.32
		243_248	3.28
		435_441	3.32
Succinic acid (2TMS)	134001	247_251	0.18
		172_176	0.55
		248_252	0.67
Citramalic acid (3TMS)	148001	115_118	0.39
		247_251	0.39
		259_264	0.20
Malic acid (3TMS)	149001	233_236	0.00
		245_249	0.39
		335_339	0.18
Citric acid (4TMS)	182004	273_278	0.23

		347_352	0.23
		465_471	0.23
Glycerol-3-phosphate (4TMS)	177002	445_448	0.10
Fructose-6-phosphate methoxyamine (6TMS)	232002	217_220	0.00
		459_462	0.00
Glucose-6-phosphate methoxyamine (6TMS)	233002	471_475	-0.32
		160_162	0.32
[644; 2-Methyl-1,3-butanediol (2TMS)]	140003	117_119	0.00
		306_309	0.36
[700; 2-methyl-1,2-propanediol (2TMS)]	141003	131_134	0.00
		292_294	0.00
		277_279	0.36
[725; 2-Ketooctanoic acid (2TMS)]	146003	185_191	0.18
		212_219	0.36
		287_294	0.18
[545; 2,3-Dimethylsuccinic acid (2TMS)]	149003	291_298	0.18
		275_281	0.18
		207_209	0.18
[815; Ethyl-3(2H)-thiophenone]	150003	128_131	0.14
[729; N,N-Dimethyllysine methyl ester]	151003	128_131	0.71
		84_88	0.00
[680; 2,3-Dimethylsuccinic acid (2TMS)]	158003	287_294	0.45
		377_384	0.23
[882; Ornithine (3TMS)]	162001	142_146	0.00
		348_353	0.43
		115_117	0.00
[548; Leucine (2TBS)]	165002	315_320	0.00
		200_203	0.00
		330_335	-0.25
[612; 4-Aminobutyric acid (2TBS)]	175003	112_118	0.23
		274_280	0.25
		376_383	0.58
[636; 4R-Acetamido-2,3-(Z)-epoxy-4-(E)-hydroxycyclohexane (1TMS)]	176005	184_189	0.23
[829; Orotic acid (3TMS)]	176003	254_258	0.25
		357_362	0.00
		269_274	-0.23
[757; 2-Desoxy-pentos-3-ylose dimethoxyamine (2TMS)]	176004	231_235	0.00
		315_321	0.61
[812; D-Xylofuranose (4TMS)]	177004	305_308	-0.15
[731; Erythrose (3TMS)]	184003	117_119	0.23

		217_220	0.23
		204_206	0.45
[826; beta-[[(5-methyl-2-thienyl)methylene]amino]-benzeneacetic acid methyl ester]	187004	241_245	0.20
		431_437	0.00
		153_157	0.23
[772; D-Glucose (5TMS)]	189005	204_206	0.10
[793; D-Galactono-1,4-lactone (4TMS)]	196004	217_220	0.00
		243_248	0.00
		361_367	0.55
[945; beta-D-Glucopyranose (5TMS)]	197002	191_192	0.00
		204_206	0.00
		217_220	0.00
[775; Dopamine (4TMS)]	200002	174_175	0.00
		317_324	0.55
		375_382	0.55
[680; Glycerol-2-phosphate (4TMS)]	203004	243_248	0.58
		258_263	0.58
		169_174	0.85
[766; beta-D-Methylglucopyranoside (4TMS)]	203003	204_206	0.00
		259_264	0.00
		319_323	0.00
[607; Putrescine (4TMS)]	204003	375_379	-0.18
[756; beta-D-Methylglucopyranoside (4TMS)]	209004	204_206	0.27
		319_323	0.27
		243_248	0.55
[662; Ribose-5-phosphate methoxyamine {BP} (5TMS)]	211004	299_299	0.00
		315_315	0.00
[648; Ethylamine (2TMS)]	216002	174_175	0.00
		217_220	0.00
		345_349	-0.27
[705; 2-Ketogluconic acid (5TMS)]	217002	437_442	0.00
		257_262	0.00
		217_220	0.27
[733; Threitol (4TMS)]	218001	217_220	0.27
[715; Erythritol (4TMS)]	226001	373_382	0.46
		217_220	0.32
[945; Uridine (3TMS)]	248002	217_220	0.32
		259_264	0.32
[644; Erythritol (4TMS)]	252002	446_454	0.64
		217_220	0.00

[895; Isomaltose methoxyamine (8TMS)]	281001	204_206 361_367	0.32 0.32
[542; Maltose methoxyamine {BP} (8TMS)]	282003	204_206	0.80

Table 3

```
NAME:13C_1731.2_1313EC11_Ribitol (5TMS)
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:173001-11-1
RI:1731
RT:10.550
NUM PEAKS:  41
( 70    3) ( 72   18) ( 73 1000) ( 74   80) ( 75   63)
( 87    8) ( 89    7) ( 90   22) (103   32) (104  189)
(105   13) (106    5) (119   83) (131   28) (132  120)
(133   70) (134   12) (146   11) (147  318) (148   50)
(149   30) (191   50) (192   20) (206   53) (207   98)
(208   18) (209    6) (220  215) (221   71) (222   20)
(223    4) (248   15) (279    9) (280    4) (281    4)
(310   23) (311    6) (322    8) (323   42) (324   12)
(325    5)

NAME:13C_1318.4_1313EC16_Proline (2TMS)
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:132003-11-1
RI:1318
RT:6.620
NUM PEAKS:  19
( 70    7) ( 71   17) ( 72   28) ( 73  600) ( 74   60)
( 80    7) ( 84    5) ( 85   17) ( 86    5) (115    6)
(128    4) (142    4) (143    3) (144   20) (145   39)
(146 1000) (147   90) (148   33) (220   38)

NAME:13C_1318.9_1313EC16_Threonine (2TMS)
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:132001-11-1
RI:1319
RT:6.627
NUM PEAKS:  58
( 73 1000) ( 75  547) ( 76   49) ( 77   23) ( 79    8)
( 81   58) ( 82    5) ( 88  115) ( 89   29) ( 90    4)
( 91    3) ( 92    3) ( 93    7) ( 96    4) (102   45)
(103   54) (104   22) (105   15) (106    4) (114    3)
(116   11) (117   80) (118   56) (119  667) (120   55)
(121   21) (129    2) (130    7) (132   40) (133  663)
(134  170) (135   38) (136    6) (149  335) (150   30)
(151   12) (153    3) (159    5) (161    7) (162   31)
(178    4) (190    2) (191    2) (192    2) (205    7)
(206   17) (207   10) (208    3) (210    2) (221  193)
(222   33) (223   27) (224    5) (225    3) (234    5)
(235    3) (252   18) (253    3)

NAME:13C_1413.9_1313EC16_
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:141004-11-1
RI:1414
RT:7.745
NUM PEAKS:  27
( 72   44) ( 73  604) ( 74  142) ( 75 1000) ( 76  120)
( 77  113) ( 87   85) ( 88   70) (103   47) (104   71)
(105   62) (106   26) (117   85) (118   29) (119  145)
(120   39) (121  447) (132  323) (133  198) (148   76)
(151   59) (160   25) (161   22) (162  190) (163   21)
(164   15) (177   23)

NAME:13C_1420.9_1313EC16_Alanine (BP) (3TMS)
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COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:142001-11-1
RI:1421
RT:7.827
NUM PEAKS: 34
(72 122) (73 1000) (74 112) (75 354) (76 29)
(87 18) (88 23) (100 78) (101 25) (102 73)
(103 27) (104 12) (115 7) (117 42) (118 517)
(119 48) (120 17) (131 20) (133 52) (134 8)
(146 38) (147 353) (148 56) (149 49) (162 420)
(163 42) (164 15) (190 15) (192 115) (193 20)
(236 20) (265 75) (266 15) (267 6)

NAME:13C_1489.8_1313EC16_Malic acid (3TMS)
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:149001-11-1
RI:1490
RT:8.637
NUM PEAKS: 59
(70 3) (72 30) (73 1000) (74 90) (75 140)
(76 9) (87 10) (101 31) (102 8) (103 53)
(104 6) (105 6) (115 10) (117 23) (118 23)
(119 9) (131 30) (132 11) (133 127) (134 17)
(135 12) (143 7) (146 10) (147 413) (148 62)
(149 46) (150 5) (151 9) (175 29) (176 9)
(177 30) (178 12) (189 19) (190 16) (191 60)
(192 20) (193 6) (206 5) (207 4) (217 8)
(220 12) (221 11) (234 7) (235 6) (236 46)
(237 8) (245 18) (249 27) (250 6) (251 4)
(263 4) (265 13) (266 11) (308 5) (309 4)
(310 9) (319 3) (323 4) (339 9)

NAME:13C_1495.3_1313EC16_
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:150003-11-1
RI:1495
RT:8.703
NUM PEAKS: 52
(72 21) (73 574) (74 66) (75 184) (76 15)
(77 11) (86 8) (87 17) (88 7) (89 6)
(95 3) (100 5) (101 37) (102 45) (103 20)
(104 15) (105 7) (115 11) (116 6) (117 26)
(118 9) (119 37) (120 3) (121 3) (129 6)
(130 47) (131 1000) (132 133) (133 81) (134 10)
(135 3) (146 3) (147 74) (148 12) (149 14)
(160 9) (161 5) (162 11) (176 4) (177 6)
(193 96) (194 8) (195 3) (204 16) (205 51)
(206 12) (207 4) (220 9) (221 3) (234 12)
(296 4) (311 3)

NAME:13C_1521.6_1313EC16_Aspartic acid (3TMS)
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:152002-11-1
RI:1522
RT:8.925
NUM PEAKS: 74
(70 7) (71 9) (72 28) (73 1000) (74 104)
(75 156) (76 11) (77 8) (84 3) (85 6)
(86 7) (87 13) (88 4) (89 5) (100 13)
(101 93) (102 157) (103 26) (104 15) (105 4)

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(115    6) (116    7) (117   17) (118   23) (119   40)
(120    4) (121    5) (130    5) (131   28) (132   42)
(133   52) (134   11) (135    7) (145   17) (146   10)
(147  157) (148   28) (149   26) (150    4) (162    3)
(163   21) (164    4) (173    3) (174    7) (175   11)
(176    9) (178    5) (189    3) (190   44) (191   11)
(192    5) (203    3) (204   40) (205   11) (206   13)
(207    4) (218    4) (219   21) (220   71) (221   18)
(222    7) (233    4) (234   20) (235  357) (236   64)
(237   30) (238    4) (248    4) (249    3) (294    5)
(309   10) (310    3) (338    5) (353    3)

NAME:13C_1594.8_1313EC16_
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:159001-11-1
RI:1595
RT:9.493
NUM PEAKS:  33
( 70   10) ( 72   58) ( 73 1000) ( 74  105) ( 75  173)
( 86   10) ( 87   21) (100   20) (101   51) (102   30)
(115   14) (117   40) (118   15) (131   20) (133   37)
(139   12) (144   17) (145   36) (146  575) (147  211)
(148   48) (174    9) (175   15) (189   15) (190  388)
(191   40) (192   14) (220  128) (221   21) (222    9)
(293   36) (294    8) (295    4)

NAME:13C_1630.8_1313EC16_Glutamic acid (3TMS)
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:163001-11-1
RI:1631
RT:9.772
NUM PEAKS:  83
( 70    7) ( 71    9) ( 72   28) ( 73 1000) ( 74   99)
( 75  255) ( 76   18) ( 85    9) ( 86   13) ( 87   29)
( 88  162) ( 89   11) ( 99    4) (100   11) (101   62)
(102   61) (103   20) (104   14) (105    5) (113    3)
(114    3) (115   30) (116   11) (117   43) (118   20)
(119   11) (129    3) (130   15) (131  331) (132   76)
(133   88) (134   16) (135    8) (144   33) (145    7)
(146    8) (147  205) (148   38) (149   56) (150    8)
(151    4) (158    5) (159   12) (160  164) (161   26)
(162   38) (163    7) (173    4) (174    4) (175    5)
(176    4) (177    3) (178    5) (189    3) (190    4)
(191    6) (205   12) (206   29) (207    7) (208    3)
(218    9) (219    6) (220   20) (221   22) (222    6)
(233    5) (234   70) (235   16) (236    7) (248    5)
(249   25) (250  438) (251   78) (252   36) (253    4)
(263    9) (279    5) (324    6) (352    3) (353   30)
(355    4) (368   15) (369    5)

NAME:13C_1640.6_1313EC16_Phenylalanine (2TMS)
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:164001-11-1
RI:1641
RT:9.848
NUM PEAKS:  69
( 70   52) ( 71    8) ( 72   19) ( 73 1000) ( 74   93)
( 75  105) ( 76    6) ( 83   12) ( 86    6) ( 87   20)
( 96   12) ( 97   17) ( 98  163) ( 99   14) (100    5)
(101  171) (104    9) (110    3) (111   13) (112    3)
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(113    3) (117    8) (118    5) (119    5) (124    3)
(125    6) (126   10) (127   11) (128   12) (132   59)
(133   33) (134    7) (135    3) (138    5) (139    8)
(140    6) (141    6) (145    4) (146    4) (147  156)
(148   30) (149   13) (153    3) (154    3) (155    3)
(159    3) (161    4) (163    9) (168   13) (169    4)
(170    5) (175    4) (184    9) (185    9) (198    3)
(199   23) (200  267) (201   24) (202    8) (205    8)
(213   10) (219   10) (220  377) (221   82) (222   33)
(223    5) (274   23) (275    7) (303    6)

NAME:13C_1707.8_1313EC16_
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:171003-11-1
RI:1708
RT:10.369
NUM PEAKS:  168
( 70    4) ( 71   26) ( 72   27) ( 73 1000) ( 74   90)
( 75  126) ( 76    6) ( 79    3) ( 80    3) ( 85   14)
( 86   12) ( 87   22) ( 88    9) ( 89  101) ( 90   12)
( 91    8) ( 92    4) ( 93    3) ( 99    4) (101   49)
(102   11) (103   36) (104   12) (105    6) (106    4)
(108    3) (113    3) (115   13) (116   10) (117   37)
(118   20) (119    7) (120    5) (121    4) (129   25)
(130    8) (132   31) (133   39) (134    7) (136    5)
(139    3) (143    9) (144    7) (145   31) (146    9)
(147  130) (148   49) (149   14) (150    6) (157    6)
(158    7) (159   72) (160   46) (161   12) (162   11)
(163   11) (164    4) (171    4) (172    3) (174    8)
(175   63) (176   14) (177   20) (183    5) (184    3)
(186    4) (188    8) (189   14) (190   12) (191    5)
(193    4) (196    4) (205    6) (206    7) (214    4)
(215    3) (216    3) (217    3) (220   13) (227    3)
(232    8) (233    7) (234    6) (235   14) (236    4)
(239    3) (245    3) (246    3) (248   21) (249   13)
(250    4) (254    3) (256    4) (260    3) (261    4)
(262    4) (268    3) (270    4) (272    3) (276   15)
(277   28) (278   15) (279  105) (280   21) (285    3)
(286    6) (290    3) (291    3) (292    7) (293    4)
(298    5) (299    5) (300    4) (306    5) (307   10)
(308    6) (309    5) (314    5) (315    3) (316    3)
(320    5) (321   11) (322    7) (328    3) (338    4)
(340    3) (342    3) (344    3) (346    4) (349    3)
(351    8) (367    4) (368    3) (370    3) (376    4)
(378    3) (379    4) (380    5) (398    3) (400    3)
(401    4) (404    3) (409    3) (425    3) (429    4)
(438    3) (449    4) (450    3) (456    4) (457    4)
(475    3) (480    5) (481    3) (483    3) (484    3)
(487    6) (488    3) (505    3) (506    3) (510    4)
(514    3) (519    3) (523    3) (531    3) (534    4)
(536    3) (537    3) (543    4)

NAME:13C_1720.2_1313EC16_
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:172005-11-1
RI:1720
RT:10.465
NUM PEAKS:  47
( 72   28) ( 73  767) ( 74  167) ( 75 1000) ( 76   86)
( 77   40) ( 78    9) ( 86   16) ( 87  224) ( 88  272)
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( 90  186) ( 91   21) ( 92    6) (101   36) (116    9)
(117  111) (118  155) (131   56) (133  189) (134   15)
(135    6) (143   64) (144   35) (145    9) (146   20)
(148   72) (149   39) (151    5) (159  269) (160  555)
(161  142) (162  121) (163   37) (164    9) (173    7)
(175    5) (176   53) (177  668) (178   59) (179   31)
(205   11) (223   14) (233   71) (234   26) (235   11)
(279    3) (280   26)

NAME:13C_1746.9_1313EC16_
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:175003-11-1
RI:1747
RT:10.672
NUM PEAKS:  13
( 72   35) ( 73 1000) ( 74   98) ( 75  217) ( 88  144)
( 89  106) (117   50) (118  371) (147  203) (190   40)
(221  108) (280  293) (281   49)

NAME:13C_1769.9_1313EC16_Glycerol-3-phosphate (4TMS)
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:177002-11-1
RI:1770
RT:10.850
NUM PEAKS:  108
( 70    5) ( 72   26) ( 73 1000) ( 74   87) ( 75  119)
( 76    8) ( 77   18) ( 79    3) ( 90    9) ( 91    5)
( 98    3) (102   14) (103  109) (104   98) (105   25)
(106    5) (107    5) (115   17) (116   20) (117   11)
(118   32) (119   25) (120    4) (121    8) (123    3)
(131   23) (132   74) (133  123) (134   52) (135   37)
(136    5) (137   13) (147  150) (148   24) (149   21)
(150    3) (151   10) (153    3) (163    3) (164    5)
(165    5) (167    4) (179    4) (181   18) (182    3)
(183    6) (193   20) (194    4) (195   18) (196    3)
(197    5) (205    3) (206   13) (207   39) (208    9)
(209    6) (210    4) (211   97) (212   15) (213    9)
(223    3) (225   20) (226    7) (227   18) (228    3)
(242   17) (243   12) (255    8) (256    3) (257   19)
(258    3) (269    4) (283    5) (284    3) (285   20)
(286    5) (298   17) (299  180) (300   49) (301   25)
(302    4) (313    3) (314   12) (315   44) (316   13)
(317    6) (329   12) (330    4) (343   13) (344    6)
(345    3) (358   19) (359  113) (360   34) (361   16)
(362    3) (372    5) (373   30) (374   10) (375    5)
(386    3) (387   12) (388    5) (389    5) (447    4)
(448   17) (449    7) (450    3)

NAME:13C_1771.0_1313EC16_
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:177003-11-1
RI:1771
RT:10.859
NUM PEAKS:  41
( 83   83) ( 87  766) (101  497) (111   47) (112   24)
(129   41) (130  121) (143   46) (159  137) (160  296)
(172   89) (173  999) (174  192) (175 1000) (176  159)
(187  117) (188   76) (201   93) (202  342) (203   62)
(216  111) (217   73) (248  155) (250   28) (260   38)
(294   27) (305   25) (306   28) (333   30) (334  204)
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(335 247) (336 98) (340 19) (350 182) (351 59)
(366 39) (411 26) (426 18) (514 20) (536 21)
(540 17)

NAME:13C_1784.2_1313EC16_Glutamine (3TMS)
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:178001-11-1
RI:1784
RT:10.961
NUM PEAKS: 88
(70 11) (71 17) (72 32) (73 1000) (74 139)
(75 301) (76 22) (77 12) (84 4) (85 23)
(86 13) (87 52) (88 14) (89 7) (90 5)
(99 5) (100 9) (101 46) (102 33) (103 13)
(105 3) (113 4) (114 3) (115 28) (116 32)
(117 64) (118 33) (119 9) (129 13) (130 12)
(131 97) (132 43) (133 111) (134 15) (135 7)
(142 3) (143 49) (144 20) (145 11) (146 22)
(147 164) (148 67) (149 37) (150 6) (157 5)
(158 17) (159 262) (160 744) (161 87) (162 32)
(163 3) (172 4) (173 3) (174 6) (175 5)
(176 3) (177 8) (188 3) (189 6) (190 13)
(191 4) (203 3) (204 3) (205 67) (206 15)
(207 6) (217 4) (218 4) (219 9) (220 19)
(221 10) (231 7) (232 5) (233 27) (234 15)
(235 12) (248 9) (249 94) (250 17) (251 7)
(262 6) (263 3) (277 5) (278 7) (305 7)
(352 15) (353 5) (367 5)

NAME:13C_1821.6_1313EC16_Ornithine (4TMS)
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:182002-11-1
RI:1822
RT:11.252
NUM PEAKS: 70
(73 736) (74 117) (85 13) (86 15) (87 130)
(88 16) (89 6) (90 6) (100 18) (101 85)
(102 54) (103 54) (104 17) (105 3) (113 6)
(114 14) (115 25) (116 26) (117 41) (128 4)
(129 9) (130 81) (131 77) (132 32) (144 19)
(145 41) (146 1000) (157 8) (158 7) (159 12)
(160 8) (161 11) (162 4) (172 3) (173 33)
(174 33) (175 333) (176 61) (177 35) (178 5)
(189 10) (190 15) (191 11) (192 8) (202 7)
(203 70) (204 19) (205 20) (206 16) (218 38)
(219 16) (220 54) (236 3) (246 7) (247 6)
(248 3) (249 7) (263 28) (264 27) (265 6)
(290 3) (320 6) (321 4) (335 9) (336 3)
(410 3) (424 4) (425 23) (426 10) (427 5)

NAME:13C_1829.5_1313EC16_Arginine (5TMS)
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:183001-11-1
RI:1830
RT:11.313
NUM PEAKS: 91
(70 25) (71 20) (72 126) (73 1000) (74 244)
(75 99) (76 7) (84 6) (85 76) (86 27)
(87 34) (88 13) (89 11) (90 13) (98 3)
(99 11) (100 73) (101 58) (102 55) (103 16)

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(104   14) (113    4) (114    6) (115   21) (116   14)
(117   57) (118   14) (123    5) (128   13) (129   32)
(130   22) (131   50) (132   36) (133   33) (134    6)
(142    4) (143   18) (144   42) (145  105) (146  201)
(147  110) (148   35) (149   10) (156    4) (157    9)
(158   14) (159   46) (160   60) (161  521) (162   59)
(163   20) (171    4) (172   35) (173   37) (174   16)
(177    9) (187    3) (188   14) (189    9) (190   10)
(191    5) (192    6) (201    3) (202    3) (203    3)
(204    4) (205    3) (217    3) (218    3) (219   17)
(220   29) (221    6) (222    3) (234    3) (235    5)
(245    8) (246    4) (248    4) (249   18) (250    3)
(259    4) (260   15) (261  189) (262   37) (263   16)
(264    6) (274    4) (289    3) (335    3) (364    5)
(379    7)

NAME:13C_1835.5_1313EC16_
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:184003-11-1
RI:1836
RT:11.359
NUM PEAKS:  91
( 71    8) ( 72   27) ( 73 1000) ( 74   86) ( 75  140)
( 76   11) ( 77    9) ( 86   13) ( 87   45) ( 88   75)
( 89   12) ( 90   37) ( 91    4) (101   21) (102   20)
(103   39) (104   73) (105   17) (106    3) (114   12)
(115   14) (116   30) (117   21) (118   38) (119  123)
(120   11) (121    4) (129    4) (130    7) (131   40)
(132   78) (133   97) (134   21) (135   10) (143    5)
(146   18) (147  251) (148   42) (149   44) (150    6)
(151    3) (157    3) (158    4) (160   44) (162   23)
(163   16) (164   16) (165    3) (175   28) (176   13)
(177   27) (178   10) (179    4) (188   11) (189   13)
(190    5) (191   45) (192   65) (193   13) (194    4)
(202    3) (203    8) (204   21) (205    6) (206   87)
(207   37) (208    9) (217    8) (218   12) (219    6)
(220   87) (221   72) (222   17) (223    5) (232   10)
(233   51) (234   14) (235   41) (236   24) (237    7)
(250    8) (263    3) (278    4) (279    3) (307    8)
(322   12) (323   10) (324    4) (337   20) (338    4)
(412    4)

NAME:13C_1843.2_1313EC16_
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:184004-11-1
RI:1843
RT:11.419
NUM PEAKS:  29
( 72   23) ( 73 1000) ( 74   79) ( 75  100) ( 89    6)
( 90   16) (102   10) (103   40) (104   57) (115    9)
(118   21) (119   59) (131   26) (132   62) (133   64)
(134   13) (147  221) (148   39) (149   25) (191   44)
(192  259) (193   43) (194   17) (206  349) (207   66)
(208   24) (220  129) (222   12) (235    5)

NAME:13C_1870.4_1313EC16_
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:187004-11-1
RI:1870
RT:11.629
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NUM PEAKS: 85
(70 10) (71 11) (72 21) (73 1000) (74 88)
(75 68) (76 3) (84 5) (85 15) (86 5)
(87 7) (90 9) (98 4) (99 8) (100 17)
(101 8) (102 6) (103 19) (104 27) (105 4)
(113 4) (114 3) (115 6) (117 6) (118 5)
(119 21) (127 7) (128 7) (129 6) (130 5)
(131 20) (133 46) (134 7) (135 4) (141 3)
(142 4) (143 8) (144 4) (145 3) (147 111)
(148 18) (149 12) (155 6) (156 11) (157 84)
(158 15) (159 8) (170 7) (171 41) (172 25)
(173 31) (175 3) (177 6) (185 5) (186 10)
(187 4) (200 5) (201 9) (202 3) (206 12)
(213 4) (214 6) (215 9) (216 3) (229 4)
(230 11) (231 5) (243 6) (244 82) (245 658)
(246 137) (247 56) (248 7) (273 11) (274 3)
(275 3) (318 3) (319 5) (347 3) (348 3)
(362 4) (436 3) (437 12) (438 5) (452 3)

NAME:13C_1879.2_1313EC16_Adenine (2TMS)
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:188005-11-1
RI:1879
RT:11.698
NUM PEAKS: 8
(73 800) (74 88) (197 207) (268 190) (269 1000)
(270 172) (283 51) (284 190)

NAME:13C_1892.4_1313EC16_Tyrosine (2TMS)
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:189006-11-1
RI:1892
RT:11.800
NUM PEAKS: 102
(70 22) (75 321) (76 26) (77 18) (79 3)
(80 3) (81 7) (82 13) (83 30) (84 29)
(85 25) (88 29) (91 8) (92 5) (93 4)
(94 3) (95 7) (96 33) (97 34) (98 56)
(99 11) (100 10) (109 5) (110 13) (111 14)
(112 16) (113 11) (114 11) (118 13) (123 7)
(124 7) (125 19) (126 28) (127 42) (128 8)
(129 6) (137 4) (138 9) (139 7) (140 14)
(141 28) (142 10) (143 9) (151 4) (152 9)
(153 5) (155 19) (156 42) (157 20) (158 5)
(166 3) (167 4) (168 9) (169 11) (170 34)
(171 15) (172 32) (173 6) (180 3) (183 14)
(184 25) (185 71) (186 1000) (187 144) (188 36)
(197 3) (198 6) (199 6) (200 19) (201 5)
(202 3) (203 5) (212 3) (213 3) (214 8)
(215 26) (216 102) (217 12) (221 48) (223 5)
(226 3) (227 12) (228 5) (229 4) (231 3)
(245 4) (260 3) (264 3) (272 3) (273 4)
(290 3) (295 3) (296 3) (301 7) (302 5)
(307 3) (317 3) (318 5) (319 32) (320 7)
(321 5) (334 4)

NAME:13C_1940.3_1313EC16_Tyrosine (3TMS)
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:194002-11-1
RI:1940

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RT:12.115
NUM PEAKS:  99
( 70    8) ( 71    6) ( 72   19) ( 73 1000) ( 74   91)
( 75  113) ( 76    7) ( 77    4) ( 82    3) ( 83    7)
( 84    6) ( 85    7) ( 86    4) ( 87   17) ( 88    3)
( 96   10) ( 97   11) ( 98   15) ( 99    3) (100    4)
(101  167) (102   27) (103   12) (104    7) (110    5)
(111    5) (112    7) (113    3) (114    3) (115    3)
(116    4) (117    6) (118    4) (119    3) (124    3)
(125    5) (126    6) (127    4) (130    3) (131   15)
(132   52) (133   25) (134    6) (137    3) (138    4)
(139    3) (140    5) (141   10) (142    3) (145    3)
(146    4) (147  109) (148   19) (149   10) (152    4)
(153    3) (154    6) (155    7) (156   19) (157    4)
(158    3) (159    3) (160    4) (161    5) (163    9)
(168    5) (169    4) (170   15) (171    8) (172    9)
(175    4) (182    3) (183    5) (184   10) (185    8)
(186   69) (187   10) (188    4) (198    3) (199    4)
(200   16) (201    3) (205    6) (214    3) (215    8)
(219   14) (220  594) (221  105) (222   50) (223    5)
(273    7) (287    9) (288   55) (289   10) (290    4)
(362   13) (363    6) (364    3) (391    6)

NAME:13C_1294.2_1313EC11_Glycerol (3TMS)
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:129003-11-1
RI:1294
RT:6.336
NUM PEAKS:  46
( 70    4) ( 71    6) ( 72   26) ( 73 1000) ( 74   89)
( 75   84) ( 76    6) ( 87   15) ( 88    7) ( 89   19)
( 90   45) (101    6) (102   14) (103   82) (104  365)
(105   39) (106   14) (118   41) (119  384) (120   31)
(132   83) (134   45) (147  644) (148  102) (149   71)
(150    9) (160    4) (161    4) (164   11) (175    5)
(176    5) (177   71) (178   42) (179   11) (180    3)
(192   31) (206   71) (207  276) (208   61) (209   26)
(220   24) (221  133) (222   26) (223   12) (265    3)
(296   18)

NAME:13C_1326.8_1313EC11_Glycine (3TMS)
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:133001-11-1
RI:1327
RT:6.720
NUM PEAKS:  59
( 70   12) ( 71    9) ( 72   26) ( 73 1000) ( 74   86)
( 75   61) ( 86   14) ( 87  313) ( 88   26) ( 89   14)
( 99    5) (100   23) (101  171) (102   32) (103   32)
(104    5) (105    5) (113    7) (114    5) (115   11)
(116   18) (117   52) (118   12) (119   13) (129    3)
(130   44) (131   52) (132   15) (133  163) (134   23)
(135   12) (147  310) (148   50) (149   24) (159   25)
(160   14) (161   16) (162    3) (173   11) (174   15)
(175  905) (176  161) (177   73) (178   14) (188    3)
(190   14) (191    3) (204   11) (205    3) (206    3)
(247    9) (248    6) (249  144) (250   39) (251   18)
(252    3) (278   44) (279   11) (280    6)

NAME:13C_1340.7_1313EC11_Succinic acid (2TMS)
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COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:134001-11-1
RI:1341
RT:6.883
NUM PEAKS: 25

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( 72   25) ( 73  546) ( 74   56) ( 75  378) ( 76   27)
( 87   13) ( 88   12) ( 89    9) (103   13) (115    8)
(116    8) (117    9) (118   25) (131   22) (132   95)
(133   51) (134   11) (147 1000) (148  159) (149   84)
(176   43) (177   20) (179    7) (251   75) (252   11)
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NAME:13C_1380.4_1313EC11_Alanine (3TMS)
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:138002-11-1
RI:1380
RT:7.350
NUM PEAKS: 50

```
( 70   25) ( 71   27) ( 72   36) ( 73  999) ( 85   23)
( 86   22) ( 99   10) (100   47) (102  790) (103   93)
(113   12) (114   10) (116  233) (117   68) (129    6)
(130   72) (131   95) (133  261) (135   18) (139    3)
(144    6) (147  370) (148   35) (158    6) (159   28)
(160   10) (161    9) (173   24) (174   28) (176   25)
(177    6) (187    3) (188    7) (189   26) (190 1000)
(191  181) (192   81) (193   24) (203    5) (233    4)
(247   11) (248    4) (263    6) (264  137) (265   38)
(266   17) (292    3) (293   28) (294    8) (295    4)
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NAME:13C_1381.6_1313EC11_Serine (3TMS)
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:138001-11-1
RI:1382
RT:7.365
NUM PEAKS: 58

```
( 70    7) ( 71   10) ( 72   27) ( 73 1000) ( 74  104)
( 75  158) ( 76   11) ( 77    6) ( 85    8) ( 86    7)
( 87   22) ( 88   11) ( 89   19) ( 90    9) (100   10)
(101  122) (103   22) (104   63) (105   10) (106    3)
(115   14) (117   25) (118   70) (119   26) (120    4)
(131   29) (132   46) (133   73) (134   24) (135    8)
(145    7) (146   11) (147  163) (148   31) (150    6)
(159    5) (160    7) (161    5) (162    6) (163    7)
(174    9) (175   10) (176    9) (177    5) (204    7)
(205   28) (206  318) (207   57) (208   25) (218    3)
(219   16) (220  169) (221   37) (222   15) (223    3)
(280   17) (281    5) (309    8)
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NAME:13C_1405.3_1313EC11_Threonine (3TMS)
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:140001-11-1
RI:1405
RT:7.644
NUM PEAKS: 71

```
( 70    6) ( 71    8) ( 72   27) ( 73 1000) ( 74  100)
( 75  135) ( 76    9) ( 77    5) ( 85    7) ( 86    6)
( 87   28) ( 88   23) ( 89    9) ( 99    3) (100    5)
(101   93) (102  167) (103   43) (104   18) (105    7)
(115   12) (116    7) (117   45) (118   20) (119  219)
(120   19) (121    8) (130   13) (131  141) (132   73)
(133   92) (134   30) (135    9) (145    8) (146    7)
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(147  153) (148   30) (149   23) (150    3) (159    6)
(160   16) (161   14) (162    6) (163    6) (173    4)
(175    8) (176    3) (177    3) (178    5) (189    7)
(190    3) (191    5) (192    7) (204    3) (205   51)
(206   17) (207    8) (219    5) (220   86) (221  309)
(222   60) (223   26) (224    3) (234    6) (292    3)
(293   53) (294   16) (295   30) (296    8) (297    3)
(324    9)

NAME:13C_1411.1_1313EC11_
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:141003-11-1
RI:1411
RT:7.711
NUM PEAKS:  27
( 71  217) ( 73  785) ( 74   54) ( 81   73) ( 85   65)
( 95   18) ( 99    9) (103   88) (110   27) (118   46)
(133  129) (134 1000) (135   90) (136   21) (147  231)
(148   38) (149   62) (150    9) (157    6) (191   18)
(192   16) (207   10) (279    9) (280    7) (294  126)
(295   28) (296   14)

NAME:13C_1440.4_1313EC11_
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:144003-11-1
RI:1440
RT:8.056
NUM PEAKS:  54
( 70    8) ( 71    9) ( 72   33) ( 73 1000) ( 74  143)
( 75  437) ( 76   41) ( 77   20) ( 85    6) ( 86    6)
( 87   16) ( 88   12) ( 89   12) ( 90    3) ( 91    6)
(100    5) (101   13) (102   67) (103   23) (104   27)
(105    4) (115    6) (116    7) (117   20) (118  262)
(119  143) (120   18) (121    4) (131   31) (132  279)
(133   59) (134   17) (146    7) (147  171) (148   46)
(149   22) (150    4) (161    4) (162   39) (163  455)
(164   40) (165   17) (175    6) (176    8) (191    5)
(204   16) (205    3) (222   13) (237   29) (238    5)
(248    8) (249   38) (250    6) (266   10)

NAME:13C_1458.8_1313EC11_Homoserine (3TMS)
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:146001-11-1
RI:1459
RT:8.273
NUM PEAKS:  67
( 70    8) ( 71   11) ( 72   31) ( 73 1000) ( 74  103)
( 75  145) ( 76   12) ( 85    9) ( 86    7) ( 87   23)
( 88   17) ( 89   10) ( 90    4) ( 95    3) (100   13)
(101   44) (102   83) (103   69) (104  223) (105   30)
(106   10) (113    3) (115   15) (116   11) (117   25)
(118   15) (119    9) (129    5) (130   23) (131  399)
(132   77) (133  112) (134   37) (135    9) (144    4)
(145    6) (146    7) (147  141) (148   28) (149   48)
(150    6) (159    4) (160    9) (161    6) (173    3)
(175    6) (176   17) (177    9) (189    3) (190    7)
(192    4) (204    7) (205   32) (206    8) (218    7)
(219   12) (220   42) (221  487) (222   84) (223   37)
(224    4) (234   22) (235    6) (236    7) (295   15)
(296    5) (324    7)
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NAME:13C_1464.4_1313EC11_
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:146003-11-1
RI:1464
RT:8.339
NUM PEAKS: 50

(70	22)	(71	24)	(72	83)	(73	580)	(75	242)
(76	18)	(77	19)	(83	4)	(84	7)	(85	32)
(86	46)	(87	10)	(88	5)	(89	4)	(99	8)
(100	22)	(101	44)	(105	4)	(113	5)	(114	5)
(115	14)	(116	7)	(129	24)	(130	14)	(133	60)
(134	9)	(135	5)	(147	1000)	(148	161)	(149	97)
(150	10)	(151	3)	(159	13)	(160	6)	(173	12)
(175	8)	(190	11)	(191	32)	(192	3)	(203	7)
(218	8)	(219	68)	(220	16)	(221	3)	(263	7)
(264	4)	(293	9)	(294	70)	(295	12)	(296	4)

NAME:13C_1467.2_1313EC11_
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:147003-11-1
RI:1467
RT:8.372
NUM PEAKS: 57

(71	42)	(73	1000)	(74	100)	(80	7)	(81	3)
(82	4)	(87	49)	(88	17)	(89	15)	(90	7)
(99	9)	(100	43)	(101	99)	(102	268)	(103	49)
(104	15)	(109	3)	(114	14)	(115	34)	(116	27)
(117	412)	(118	43)	(119	20)	(128	7)	(130	60)
(131	667)	(132	92)	(142	15)	(143	11)	(144	34)
(145	307)	(146	57)	(154	11)	(157	11)	(158	57)
(159	26)	(160	13)	(161	5)	(162	5)	(172	9)
(174	185)	(175	25)	(176	18)	(188	3)	(189	9)
(205	20)	(216	2)	(217	3)	(232	9)	(233	3)
(246	8)	(247	17)	(248	188)	(249	32)	(250	13)
(262	5)	(263	16)						

NAME:13C_1473.2_1313EC11_
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:147002-11-1
RI:1473
RT:8.442
NUM PEAKS: 64

(74	1000)	(77	3)	(78	3)	(80	3)	(85	6)
(86	7)	(87	5)	(88	7)	(89	6)	(90	50)
(91	5)	(94	4)	(101	40)	(102	25)	(105	3)
(110	3)	(114	3)	(115	4)	(116	4)	(117	32)
(122	3)	(130	5)	(131	10)	(132	36)	(142	4)
(145	8)	(146	146)	(157	3)	(158	7)	(159	5)
(160	4)	(162	5)	(163	37)	(164	7)	(174	10)
(176	23)	(186	3)	(188	5)	(191	5)	(194	4)
(210	3)	(215	3)	(220	14)	(228	3)	(245	3)
(280	4)	(323	3)	(335	4)	(349	3)	(360	3)
(385	3)	(386	4)	(387	3)	(410	3)	(423	3)
(431	4)	(434	3)	(441	3)	(459	3)	(495	3)
(524	4)	(532	3)	(535	3)	(542	3)		

NAME:13C_1481.0_1313EC11_
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:148002-11-1

RI:1481
RT:8.534
NUM PEAKS: 16
(71 19) (73 1000) (85 62) (87 47) (101 44)
(102 59) (103 15) (104 31) (143 143) (147 273)
(149 21) (158 34) (159 985) (160 91) (161 30)
(233 55)

NAME:13C_1503.6_1313EC11_Erythritol (4TMS)
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:150002-11-1
RI:1504
RT:8.786
NUM PEAKS: 56
(73 1000) (74 74) (75 50) (76 3) (87 4)
(89 11) (90 29) (103 54) (104 186) (105 20)
(106 5) (115 5) (116 7) (119 154) (120 11)
(121 5) (131 16) (132 68) (133 94) (134 15)
(135 8) (145 3) (146 5) (147 347) (148 55)
(149 33) (150 3) (177 6) (178 3) (189 3)
(191 67) (192 56) (193 12) (194 3) (205 4)
(206 72) (207 114) (208 22) (209 8) (218 3)
(219 12) (220 220) (221 53) (222 19) (223 3)
(235 7) (279 6) (280 3) (295 12) (296 4)
(309 5) (310 17) (311 5) (312 3) (324 6)
(325 3)

NAME:13C_1506.4_1313EC11_
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:151002-11-1
RI:1506
RT:8.808
NUM PEAKS: 68
(75 501) (76 44) (87 77) (93 13) (101 233)
(102 965) (115 44) (116 44) (117 1000) (122 8)
(123 16) (130 46) (131 727) (145 50) (157 24)
(158 28) (159 114) (161 10) (185 36) (186 16)
(190 15) (197 17) (199 12) (203 73) (204 35)
(210 10) (218 20) (227 17) (235 18) (238 14)
(242 11) (243 20) (244 9) (246 48) (247 434)
(248 74) (249 20) (250 8) (269 13) (270 12)
(275 24) (276 15) (281 13) (282 22) (305 10)
(313 10) (325 10) (339 10) (346 16) (347 11)
(350 14) (356 10) (360 13) (361 9) (368 7)
(376 11) (405 14) (426 8) (436 9) (440 10)
(448 9) (453 12) (454 17) (464 10) (518 10)
(524 7) (542 10) (553 6)

NAME:13C_1513.8_1313EC11_
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:151003-11-1
RI:1514
RT:8.865
NUM PEAKS: 67
(70 12) (72 37) (73 1000) (74 116) (75 276)
(76 21) (77 12) (85 14) (86 26) (87 59)
(88 909) (89 209) (90 21) (91 15) (100 14)
(101 79) (102 147) (103 23) (104 28) (105 32)
(106 5) (114 4) (115 18) (116 8) (117 49)
(118 17) (119 10) (120 19) (130 7) (131 102)

(132 53) (133 60) (134 11) (135 5) (144 46)
(145 10) (146 13) (147 159) (148 36) (149 17)
(158 7) (159 7) (160 118) (161 18) (162 38)
(163 17) (174 8) (175 5) (176 27) (177 5)
(190 9) (191 55) (192 885) (193 87) (194 34)
(205 22) (206 7) (218 4) (219 3) (220 17)
(221 7) (234 31) (266 14) (279 23) (280 4)
(295 10) (310 10)

NAME:13C_1528.8_1313EC11_Pyroglutamic acid (2TMS)
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:153002-11-1
RI:1529
RT:8.981
NUM PEAKS: 56
(70 20) (71 33) (72 36) (73 955) (75 138)
(76 9) (77 5) (84 7) (85 27) (86 24)
(87 21) (88 24) (95 7) (99 5) (100 7)
(101 24) (104 4) (105 4) (113 6) (114 4)
(115 31) (116 8) (117 25) (118 6) (124 14)
(130 5) (131 22) (132 9) (133 38) (134 6)
(135 3) (143 4) (144 29) (145 11) (147 167)
(148 27) (149 17) (157 3) (158 16) (159 42)
(160 1000) (161 89) (162 38) (173 4) (191 4)
(218 12) (232 4) (233 4) (234 83) (235 14)
(236 6) (262 6) (263 72) (264 12) (265 6)
(278 3)

NAME:13C_1537.7_1313EC11_
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:154002-11-1
RI:1538
RT:9.050
NUM PEAKS: 66
(72 26) (73 543) (74 85) (75 685) (76 58)
(77 35) (86 15) (87 66) (88 1000) (89 26)
(90 6) (91 6) (100 6) (101 10) (102 10)
(103 26) (104 22) (105 5) (115 13) (116 6)
(117 14) (118 44) (119 21) (120 3) (131 17)
(132 47) (133 58) (134 13) (135 5) (143 3)
(144 45) (145 7) (146 14) (147 81) (148 44)
(149 25) (150 4) (158 3) (159 4) (160 76)
(161 24) (162 225) (163 24) (164 10) (176 8)
(177 39) (178 440) (179 41) (180 17) (190 8)
(191 78) (192 6) (193 3) (206 21) (207 3)
(218 3) (234 43) (235 8) (236 4) (252 17)
(253 3) (263 6) (280 3) (281 39) (282 7)
(283 3)

NAME:13C_1561.1_1313EC11_Phenylalanine (1TMS)
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:157001-11-1
RI:1561
RT:9.232
NUM PEAKS: 85
(70 121) (72 29) (73 590) (74 118) (75 345)
(76 35) (77 17) (81 9) (83 87) (87 31)
(89 22) (91 36) (92 5) (96 25) (97 29)
(98 260) (99 31) (100 33) (101 39) (102 16)
(104 38) (108 4) (110 17) (111 101) (113 7)

(116 7) (118 28) (121 3) (124 5) (125 15)
(126 44) (127 106) (128 1000) (129 4) (132 186)
(133 42) (134 19) (138 3) (139 18) (140 5)
(143 9) (145 5) (148 414) (149 40) (150 22)
(154 4) (158 4) (159 63) (161 7) (169 9)
(174 3) (175 14) (177 4) (184 13) (185 13)
(200 3) (202 8) (213 33) (214 6) (218 4)
(220 56) (221 15) (222 63) (223 9) (224 5)
(230 3) (231 19) (232 3) (235 3) (237 4)
(244 3) (251 7) (286 3) (296 3) (303 3)
(304 3) (396 5) (397 4) (403 3) (449 3)
(470 3) (500 3) (506 3) (544 3) (565 3)

NAME:13C_1575.2_1313EC11_
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:157002-11-1
RI:1575
RT:9.341
NUM PEAKS: 57
(72 34) (73 1000) (74 121) (75 221) (76 16)
(77 8) (86 3) (89 7) (102 8) (103 39)
(105 6) (111 5) (115 6) (118 29) (119 11)
(131 25) (132 9) (133 75) (134 10) (135 6)
(145 5) (146 52) (147 430) (148 119) (149 87)
(150 12) (151 5) (161 6) (162 62) (163 9)
(175 8) (176 3) (177 4) (178 13) (191 10)
(192 109) (193 19) (194 7) (207 4) (221 19)
(222 13) (235 4) (236 35) (237 6) (266 27)
(267 8) (280 7) (281 89) (282 16) (283 6)
(294 8) (308 6) (310 8) (355 4) (383 3)
(384 12) (385 5)

NAME:13C_1580.5_1313EC11_
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:158002-11-1
RI:1581
RT:9.382
NUM PEAKS: 104
(109 37) (110 25) (111 46) (112 30) (122 61)
(123 71) (124 68) (125 82) (126 60) (127 104)
(128 25) (185 88) (186 1000) (187 69) (201 90)
(271 13) (273 13) (274 22) (275 84) (276 11)
(287 20) (289 11) (290 89) (291 20) (346 12)
(347 17) (360 14) (362 24) (363 18) (364 28)
(365 31) (366 12) (371 19) (379 10) (392 14)
(398 19) (402 20) (437 15) (438 18) (439 19)
(440 12) (441 19) (442 16) (445 22) (446 11)
(447 25) (448 10) (449 19) (450 40) (451 27)
(455 31) (456 21) (457 29) (458 29) (459 30)
(461 39) (463 27) (464 23) (465 27) (466 30)
(467 38) (469 29) (470 25) (471 20) (472 24)
(473 43) (474 32) (476 28) (477 16) (478 29)
(479 17) (480 18) (482 31) (483 18) (486 21)
(488 26) (489 20) (492 18) (493 12) (495 26)
(496 33) (498 20) (500 17) (502 14) (503 13)
(504 27) (505 22) (510 15) (513 15) (514 29)
(515 20) (517 18) (527 15) (529 16) (532 21)
(533 14) (538 14) (540 17) (542 20) (543 16)
(548 17) (549 21) (555 14) (558 10)

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NAME:13C_1581.9_1313EC11_
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:158003-11-1
RI:1582
RT:9.393
NUM PEAKS:  86
( 70    8) ( 71    9) ( 72   48) ( 73 1000) ( 74  160)
( 75  299) ( 76   16) ( 85    4) ( 86    6) ( 87    9)
( 91   25) (100    3) (101   22) (102    9) (103   28)
(104    5) (105    4) (115    8) (116    3) (117   49)
(118   42) (119   45) (130    8) (131   33) (133  100)
(134   14) (135    9) (145    4) (146   17) (147  386)
(148   86) (149   84) (150   12) (151    5) (161    7)
(162   70) (163   20) (164    5) (175   15) (176    5)
(177    8) (178    3) (190    3) (191   40) (192   12)
(193    6) (204    3) (205    3) (206    7) (207    9)
(219    6) (220   51) (221   32) (222   11) (223    6)
(234    6) (235    4) (236   38) (237   10) (238    4)
(249    4) (250    4) (263    8) (264    5) (265   41)
(266   24) (267    7) (280   12) (281  161) (282   30)
(283   14) (293    3) (294   27) (295    5) (296    4)
(308    6) (309    3) (353   12) (354    5) (355   16)
(356    6) (357    3) (383    3) (384   22) (385    7)
(386    3)
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NAME:13C_1623.1_1313EC11_
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:162001-11-1
RI:1623
RT:9.712
NUM PEAKS:  90
( 70    9) ( 71   13) ( 72   63) ( 73 1000) ( 74  759)
( 75  136) ( 76   14) ( 84    3) ( 85   16) ( 86   12)
( 87   23) ( 88   13) ( 89   37) ( 90    8) ( 91    3)
( 99    5) (100   15) (101   54) (102   80) (103  118)
(104   24) (105   11) (110    3) (113    3) (114    6)
(115   13) (116   15) (117   88) (118   26) (119   28)
(120    3) (129    4) (130   26) (131   83) (132   59)
(133   42) (134   10) (135    3) (143    3) (144   15)
(145   37) (146  650) (147  215) (148   66) (149   17)
(150    3) (157    4) (158   17) (159   16) (160    8)
(161   11) (162   61) (163   13) (164    6) (173   10)
(174   18) (175   14) (176    7) (177    4) (189    5)
(190    9) (191   10) (192    6) (203    6) (204    3)
(205    6) (206   42) (207    8) (208    3) (218    7)
(219   14) (220   47) (221   15) (222    5) (232    4)
(233    4) (234    4) (235    8) (236    8) (246    4)
(247    4) (248   31) (249   25) (263    8) (264   11)
(265    3) (352    3) (353   26) (354    8) (355    4)
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NAME:13C_1652.1_1313EC11_
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:165002-11-1
RI:1652
RT:9.937
NUM PEAKS:  30
( 73 1000) ( 74   90) ( 85   29) ( 87   28) (101   53)
(115   94) (116   75) (117   31) (129   25) (130   62)
(131   57) (144   26) (145   14) (146  115) (147  159)
(158   27) (159   26) (173   81) (174   40) (202   21)
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(203  244) (204   48) (205   17) (217   20) (232   24)
(319   17) (320  165) (321   41) (322   17) (335   14)

NAME:13C_1659.1_1313EC11_
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:166002-11-1
RI:1659
RT:9.991
NUM PEAKS:  24
( 70   15) ( 71   66) ( 72   17) ( 73 1000) ( 74   74)
( 90   26) ( 99   14) (103   36) (104  137) (113   15)
(119  132) (131   28) (132   39) (133   76) (147  266)
(148   36) (161   16) (173   36) (191   58) (203   85)
(206  309) (207  116) (208   32) (220   52)

NAME:13C_1670.3_1313EC11_Arabinose methoxyamine (4TMS)
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer |RI:1670 |RI:1670 |RI:1670
CASNO:167002-11-1
RI:1670
RT:10.078
SOURCE:C:\KOPKA\AMDIS32\LIB\File2.msp
NUM PEAKS:  63
( 71   18) ( 73 1000) ( 74   76) ( 88   12) ( 90   17)
(103   60) (104  402) (105   56) (106   16) (119   44)
(120    9) (121    7) (131   35) (132   57) (133   84)
(134   45) (135    9) (147  227) (148   39) (149   25)
(150    5) (161   12) (162   43) (163   19) (164    8)
(174    7) (177   14) (190    5) (191   61) (192   25)
(193    9) (203   10) (205    7) (206   22) (207   28)
(208   11) (216    4) (217   16) (219   12) (220  206)
(221   43) (222   21) (235   19) (237    5) (240    4)
(261    7) (265   11) (275    5) (282    3) (298    4)
(307    7) (310   73) (311   22) (312   11) (371    5)
(440    6) (477    5) (493    4) (504    4) (522    5)
(523    4) (568    3) (584    3)

NAME:13C_1683.3_1313EC11_Asparagine (3TMS)
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:168001-11-1
RI:1683
RT:10.179
NUM PEAKS:  90
( 70   10) ( 71   19) ( 72   41) ( 73 1000) ( 74  145)
( 75  265) ( 76   21) ( 77   12) ( 84    5) ( 85   11)
( 86   10) ( 87   17) ( 88    8) ( 89    5) ( 90    7)
( 99    4) (100   18) (101   69) (102   71) (103   19)
(115    9) (116   30) (117   54) (118  391) (119   39)
(120   18) (128   12) (129    3) (130   12) (131   42)
(132   47) (133  102) (134  195) (135   23) (136    7)
(143    9) (144  119) (145   21) (146   25) (147  160)
(148   29) (149   27) (150    4) (158    4) (159    5)
(160    4) (161    5) (162   46) (163    7) (164    3)
(172    3) (173   18) (174    9) (175   10) (176    4)
(177    3) (188    4) (189  108) (190   32) (191   12)
(192    8) (202    5) (203    3) (204   35) (205   11)
(206   14) (207    3) (208    3) (216    4) (217    4)
(218   20) (219   12) (220   31) (221    7) (222    3)
(232    4) (233   10) (234  146) (235   28) (236   13)
(246    3) (247    9) (248    4) (249    4) (262   26)
(263    8) (264    3) (320    4) (337    7) (352    6)
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NAME:13C_1713.4_1313EC11_
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer |RI:1713 |RI:1713
CASNO:171008-11-1
RI:1713
RT:10.412
SOURCE:C:\KOPKA\AMDIS32\LIB\File2.msp
NUM PEAKS:  115
( 73 1000) ( 74  100) ( 90   38) ( 92    9) (104  419)
(105   30) (106   13) (107    7) (118   17) (119  145)
(120   11) (132  179) (137    6) (165    7) (177   13)
(180    7) (191   48) (192   41) (193    8) (194    4)
(206   48) (207  173) (208   35) (209   14) (213    8)
(220  500) (221  137) (222   54) (223   11) (224    6)
(225    9) (227    8) (238    7) (240    6) (248   35)
(249   12) (253    4) (265   10) (267    7) (270    5)
(279   17) (280    8) (282    6) (283    4) (284    4)
(286    6) (289    9) (294   13) (295    8) (296    8)
(308    8) (309   16) (310   68) (311   24) (312   15)
(313    7) (314    7) (316    7) (321    9) (322   12)
(323   57) (324   24) (325   10) (326    5) (329    7)
(330    4) (336    5) (339    7) (344    4) (346    4)
(347    5) (349    6) (353    7) (355    9) (359    7)
(377    6) (383    8) (388    5) (390    5) (391    4)
(392    7) (393    5) (398    8) (399    8) (400    5)
(402    4) (406    4) (407    6) (408    5) (410    6)
(413    7) (416    9) (427    4) (431    5) (452    6)
(454    7) (458    6) (459   13) (464    4) (466    9)
(476    4) (479    5) (482    3) (488    6) (490    4)
(493    5) (498    8) (502    4) (503    6) (508    7)
(509    4) (524    7) (558    7) (567    6) (596    3)

NAME:13C_1758.0_1313EC11_
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:176005-11-1
RI:1758
RT:10.758
NUM PEAKS:  108
( 70   54) ( 71   49) ( 72  115) ( 73  588) ( 74 1000)
( 75  240) ( 76   25) ( 77   13) ( 79   10) ( 80    3)
( 81    3) ( 83    6) ( 84   12) ( 85   92) ( 86   33)
( 87   45) ( 88   46) ( 89  129) ( 90   23) ( 91    6)
( 92    3) ( 93    5) ( 94    3) ( 95    3) ( 97    4)
( 98    7) ( 99   31) (100  145) (101   43) (102   33)
(103   14) (104   26) (105    7) (106    3) (109    3)
(111    4) (112    4) (113    9) (114    7) (115   28)
(116   25) (117   26) (118   29) (119    6) (124    3)
(125    3) (126    3) (127    7) (128   33) (129   40)
(130   13) (131   27) (132   58) (133   39) (134    7)
(135    4) (140    3) (141    4) (142    3) (143   24)
(144   23) (145   42) (147   55) (148   26) (149   12)
(150    3) (156    5) (157    8) (158   10) (159   19)
(160   12) (161   10) (162   22) (163    7) (164    3)
(169    4) (171    4) (172   18) (173   35) (174   11)
(177   71) (178    6) (179    5) (187    8) (188   38)
(189  364) (190   40) (191   44) (192   14) (193    3)
(202    5) (203    3) (211    6) (215    4) (216    3)
(217    9) (218    4) (219    3) (229    8) (230    3)
(263   10) (264    4) (275    4) (285    3) (290    3)
(291    3) (292    8) (307    3)
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NAME:13C_1763.8_1313EC11_Ornithine (3TMS); Arginine (BP) (3TMS)
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:176006-11-1
RI:1764
RT:10.803
NUM PEAKS: 81

(70 11)	(71 13)	(72 84)	(73 1000)	(74 297)
(75 200)	(76 18)	(77 7)	(84 4)	(85 19)
(86 17)	(87 211)	(88 39)	(89 13)	(90 16)
(91 4)	(99 5)	(100 28)	(101 102)	(102 47)
(103 40)	(104 13)	(105 4)	(113 8)	(114 12)
(115 18)	(116 23)	(117 32)	(118 18)	(119 11)
(129 5)	(130 78)	(131 77)	(132 41)	(133 44)
(134 7)	(135 3)	(143 3)	(144 11)	(145 15)
(146 261)	(147 141)	(148 48)	(149 16)	(150 3)
(157 5)	(158 9)	(159 29)	(160 8)	(161 24)
(162 39)	(163 5)	(173 20)	(174 35)	(175 707)
(176 127)	(177 75)	(178 8)	(190 15)	(191 200)
(192 32)	(193 9)	(203 11)	(204 4)	(205 3)
(206 5)	(218 4)	(219 5)	(220 29)	(221 7)
(222 3)	(248 12)	(249 55)	(250 10)	(251 4)
(263 16)	(264 5)	(352 4)	(353 32)	(354 10)
(355 4)				

NAME:13C_1774.2_1313EC11_
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:177004-11-1
RI:1774
RT:10.884
NUM PEAKS: 50

(72 17)	(73 1000)	(74 81)	(75 72)	(76 10)
(86 12)	(90 6)	(100 4)	(114 5)	(115 9)
(116 8)	(119 14)	(131 33)	(132 38)	(133 51)
(144 3)	(145 9)	(146 30)	(147 249)	(148 41)
(149 31)	(150 4)	(161 6)	(164 6)	(174 23)
(178 3)	(192 29)	(205 3)	(206 14)	(219 17)
(220 481)	(221 105)	(222 43)	(223 6)	(235 45)
(236 11)	(237 4)	(248 7)	(249 6)	(250 3)
(261 3)	(262 13)	(263 4)	(295 6)	(308 13)
(309 4)	(322 4)	(455 4)	(456 12)	(457 6)

NAME:13C_1794.5_1313EC11_
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:179002-11-1
RI:1795
RT:11.041
NUM PEAKS: 162

(70 14)	(72 26)	(75 306)	(76 47)	(80 8)
(82 13)	(85 28)	(86 32)	(87 461)	(90 19)
(92 13)	(95 16)	(100 20)	(101 158)	(103 58)
(113 26)	(122 10)	(124 13)	(126 10)	(129 16)
(130 39)	(141 10)	(143 14)	(144 19)	(146 33)
(154 12)	(160 115)	(161 74)	(171 23)	(175 1000)
(176 168)	(177 62)	(178 27)	(180 10)	(181 13)
(182 16)	(187 19)	(188 16)	(191 91)	(192 23)
(196 14)	(199 9)	(212 11)	(213 15)	(214 15)
(215 10)	(224 11)	(226 8)	(232 10)	(233 18)
(239 12)	(241 7)	(244 12)	(245 12)	(247 15)
(250 15)	(256 13)	(257 14)	(258 16)	(259 12)

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(260   21) (262   21) (266   13) (269   10) (272   10)
(273    7) (274   11) (275   10) (276   12) (277   19)
(288   18) (289    7) (290   19) (291    7) (296   12)
(308   13) (309    9) (311   10) (312    8) (316   11)
(317   18) (318   23) (322   13) (324   11) (332   18)
(335   14) (337   14) (339   10) (340    8) (346    9)
(349   18) (350   81) (351   30) (352   15) (357   10)
(369   11) (370    9) (372   13) (373   13) (374   13)
(379   11) (380   12) (383    9) (384   15) (385    9)
(386   22) (390   12) (398    8) (404   16) (406    8)
(407   13) (413    9) (414   14) (421   14) (423   25)
(424   20) (426    9) (427   17) (433    9) (435    8)
(438   12) (447    9) (453   12) (456   13) (463   11)
(464   13) (466    9) (468    9) (470   14) (471   12)
(476   12) (477   21) (478   11) (480   12) (481   12)
(482   14) (483   14) (487   10) (490   14) (494    8)
(496   12) (503   19) (510   17) (511   12) (513   17)
(515   11) (517   11) (522   15) (524   17) (525    9)
(530   11) (534   13) (537   12) (546    9) (547    9)
(549    9) (555    8) (565   11) (567   11) (571   12)
(577    5) (593    4)

NAME:13C_1809.0_1313EC11_
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:181005-11-1
RI:1809
RT:11.153
NUM PEAKS:  13
( 73 1000) (118   18) (119   58) (131   53) (133   66)
(147  162) (148   33) (192  423) (193   87) (206  721)
(207  121) (208   38) (220  107)

NAME:13C_1813.5_1313EC11_Glyceric acid-3-phosphate (4TMS)
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:181003-11-1
RI:1814
RT:11.189
NUM PEAKS:  40
( 72   21) ( 73 1000) ( 74   81) ( 75  106) ( 77   14)
(103   96) (105   12) (117    8) (118   29) (119   23)
(121    8) (131   22) (133  111) (134   13) (135   35)
(147  233) (148   40) (149   21) (181   18) (191   24)
(193   20) (195   17) (211  130) (212   19) (225   18)
(227  101) (228   15) (255    8) (285   15) (299  137)
(300   35) (315   47) (316   14) (358   12) (359   68)
(360   18) (361    8) (387   32) (388   14) (462   15)

NAME:13C_1852.0_1313EC11_
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:185004-11-1
RI:1852
RT:11.487
NUM PEAKS:  33
( 75 1000) ( 76  100) ( 77   67) ( 81   48) (118  188)
(119  463) (129  239) (131   85) (132  469) (134  270)
(135   49) (143   33) (145  114) (150   20) (153   19)
(163   32) (192   29) (205   47) (208   25) (213   22)
(239   12) (286   49) (299  109) (312   19) (334   18)
(379   20) (380   13) (382   16) (412   17) (413   17)
(441   22) (462   12) (483   17)
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NAME:13C_1878.9_1313EC11_alpha-D-Methylglucopyranoside (4TMS)
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:188006-11-1
RI:1879
RT:11.695
NUM PEAKS:  45
( 73 1000) ( 74   100) ( 76    41) ( 77    11) ( 93    16)
( 96    2) ( 97     2) (100     6) (113     3) (118    35)
(121   13) (122     5) (123     3) (127     2) (134   235)
(135   26) (136     8) (150    39) (151     4) (167    13)
(168    3) (169     3) (171     2) (174    17) (179     2)
(189    9) (196     2) (197     6) (205    20) (206   500)
(223   22) (224     3) (245     9) (246     2) (247     2)
(250    3) (268     7) (269    33) (270     6) (271     2)
(277    4) (284     5) (293    10) (351     2) (383     4)

NAME:13C_1882.2_1313EC11_Mannose methoxyamine (5TMS)
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:188002-11-1
RI:1882
RT:11.721
NUM PEAKS:  62
( 70    6) ( 72    18) ( 73  1000) ( 74    84) ( 75   136)
( 87   37) ( 88    20) ( 90    13) (101    29) (102    16)
(105   27) (114     3) (115    24) (117    18) (119    78)
(120    5) (130    15) (131    75) (132   112) (133    43)
(144    8) (145    11) (147   343) (148    37) (160    70)
(161  116) (162   170) (163    26) (164     7) (178     6)
(203   10) (207   173) (208    20) (209    13) (210     3)
(211    7) (216     4) (219    13) (232     5) (233    29)
(234   49) (235    14) (236     7) (251     3) (260     3)
(278    6) (294    22) (295     5) (296     5) (299    11)
(308    3) (321     4) (322    31) (323   167) (324    51)
(325   20) (341     4) (359     8) (370     4) (373     5)
(469    3) (514     4)

NAME:13C_1888.8_1313EC11_
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:189005-11-1
RI:1889
RT:11.772
NUM PEAKS:  5
(192  571) (193    87) (194    40) (206  1000) (441     7)

NAME:13C_1893.5_1313EC11_Glucose methoxyamine (5TMS)
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:189002-11-1
RI:1894
RT:11.808
NUM PEAKS:  91
( 70    6) ( 71     6) ( 72    17) ( 73  1000) ( 74    98)
( 75   91) ( 76     4) ( 85     5) ( 86    10) ( 87    33)
( 88    6) ( 89    45) ( 90    33) ( 91     5) (100     3)
(101   22) (102    16) (103    42) (104   131) (105    53)
(106   10) (114     4) (115    11) (116    24) (117    15)
(118   14) (119   126) (120    11) (121     5) (129     4)
(130   10) (131    46) (132   186) (133   106) (134    39)
(135   10) (144     4) (145    12) (146    24) (147   486)
(148   82) (149    48) (150     6) (159     4) (160     9)
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(161  126) (162  232) (163   49) (164   17) (173    6)
(174    6) (175    4) (176    7) (177    9) (178    6)
(189    4) (190    7) (191   52) (193    7) (203    6)
(204    5) (205    6) (207  240) (208   47) (209   22)
(218    5) (219   18) (220  131) (221   38) (222   15)
(223    3) (232    3) (233   39) (234   19) (235   23)
(236    8) (237    3) (247    3) (248    7) (249    6)
(250    4) (261    3) (264    3) (275    4) (306    3)
(308    6) (310    5) (322   14) (323  188) (368    5)
(380    3)
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NAME:13C_1914.8_1313EC11_Glucose methoxyamine (BP) (5TMS)
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:191001-11-1
RI:1915
RT:11.953
NUM PEAKS: 68

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( 73 1000) ( 75   54) ( 87   18) ( 89   67) ( 90   29)
( 91    5) (101   17) (103   31) (104  208) (105   37)
(106   10) (118   11) (119   92) (120   10) (121    4)
(132  126) (133   76) (134   38) (135    9) (145    5)
(147  332) (148   54) (149   35) (150    4) (161   85)
(162  133) (163   31) (164   10) (173    4) (177    8)
(178    6) (190    6) (191   36) (192   16) (193    5)
(203    3) (204    3) (205    5) (206   40) (207  188)
(208   36) (209   16) (219    8) (220   86) (221   24)
(222   10) (233   26) (234    8) (235   22) (236    7)
(237    9) (248    5) (249    4) (250    3) (274    3)
(278    5) (279    8) (280    3) (294   10) (295    3)
(308    5) (309    3) (310    5) (322   12) (323  159)
(324   46) (325   23) (326    4)
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NAME:13C_1931.9_1313EC11_Sorbitol (6TMS); Glucitol (6TMS)
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:193001-11-1
RI:1932
RT:12.062
NUM PEAKS: 79

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( 71    4) ( 72   20) ( 73 1000) ( 74   85) ( 75   68)
( 76    4) ( 87   17) ( 88    5) ( 89    9) ( 90   28)
( 91    3) (102   11) (103   33) (104  179) (105   19)
(106    7) (115    5) (116    5) (117    7) (118   10)
(119  107) (120    8) (121    4) (131   27) (132   92)
(133   73) (134   12) (135    6) (145    4) (146   14)
(147  344) (148   59) (149   35) (150    4) (160    8)
(161   73) (162    7) (163    5) (164    4) (177    7)
(178    3) (189   10) (191   39) (192   35) (193    9)
(205    6) (206   50) (207  157) (208   29) (209   12)
(219    6) (220  165) (221   40) (222   16) (223    3)
(233   16) (234    7) (235   17) (236    3) (261    7)
(264    5) (279    8) (280    4) (294    8) (308    6)
(309    8) (310   26) (311    7) (312    3) (322   12)
(323  127) (324   36) (325   17) (326    3) (336   10)
(337    3) (351    6) (425    3) (426    4)
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NAME:13C_1956.1_1313EC11_
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:196004-11-1
RI:1956
RT:12.216

NUM PEAKS: 94

(70 4)	(72 20)	(73 1000)	(74 92)	(75 122)
(76 9)	(77 9)	(86 29)	(87 12)	(88 6)
(89 35)	(90 26)	(91 7)	(100 3)	(101 12)
(102 13)	(103 32)	(104 99)	(105 21)	(106 5)
(114 6)	(115 17)	(116 9)	(117 11)	(118 14)
(119 59)	(120 6)	(129 4)	(130 7)	(131 28)
(132 116)	(133 74)	(134 18)	(135 8)	(144 8)
(145 12)	(146 19)	(147 174)	(148 36)	(149 46)
(150 5)	(151 3)	(158 5)	(159 5)	(160 15)
(162 18)	(163 21)	(164 4)	(173 7)	(174 57)
(175 32)	(176 12)	(177 12)	(178 4)	(190 10)
(191 36)	(192 24)	(193 6)	(203 3)	(204 3)
(205 6)	(206 57)	(207 21)	(208 7)	(218 4)
(219 12)	(220 226)	(221 43)	(222 30)	(223 5)
(232 3)	(233 6)	(234 6)	(235 6)	(246 3)
(247 7)	(248 32)	(249 12)	(250 5)	(251 5)
(264 5)	(265 3)	(277 17)	(278 4)	(294 4)
(308 4)	(323 7)	(336 6)	(337 13)	(338 5)
(366 7)	(367 41)	(368 13)	(369 6)	

NAME:13C_1973.5_1313EC11_
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:197002-11-1
RI:1974
RT:12.326
NUM PEAKS: 61

(70 4)	(72 19)	(73 1000)	(74 86)	(75 97)
(77 3)	(86 9)	(87 9)	(88 4)	(90 13)
(101 5)	(102 8)	(103 34)	(104 59)	(105 9)
(106 3)	(114 3)	(115 8)	(117 8)	(118 17)
(119 36)	(120 3)	(131 27)	(132 67)	(133 67)
(134 11)	(135 6)	(145 4)	(146 17)	(147 227)
(148 37)	(160 7)	(161 11)	(164 3)	(176 3)
(177 4)	(178 3)	(189 3)	(191 47)	(192 270)
(193 47)	(194 20)	(204 8)	(205 13)	(206 441)
(207 81)	(208 36)	(209 4)	(220 84)	(221 28)
(222 11)	(234 3)	(235 9)	(236 4)	(248 6)
(294 6)	(308 6)	(322 3)	(323 4)	(351 3)
(441 3)				

NAME:13C_1999.9_1313EC11_Gluconic acid (6TMS)
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:200001-11-1
RI:2000
RT:12.494
NUM PEAKS: 62

(73 1000)	(81 19)	(82 28)	(90 16)	(96 19)
(98 15)	(103 22)	(104 95)	(105 13)	(109 5)
(112 12)	(119 66)	(124 6)	(125 22)	(127 4)
(132 63)	(133 65)	(134 11)	(135 8)	(147 349)
(148 57)	(149 38)	(161 26)	(168 5)	(191 39)
(192 23)	(206 40)	(207 68)	(208 13)	(209 7)
(220 87)	(221 28)	(222 17)	(233 7)	(248 9)
(249 7)	(261 4)	(266 4)	(279 14)	(294 67)
(295 23)	(296 11)	(308 29)	(309 13)	(310 11)
(311 5)	(323 29)	(336 18)	(337 64)	(338 23)
(339 12)	(340 6)	(344 5)	(346 6)	(350 5)
(364 8)	(365 14)	(428 5)	(454 4)	(505 7)
(528 4)	(550 4)			

NAME:13C_2026.0_1313EC11_
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:203003-11-1
RI:2026
RT:12.660
NUM PEAKS: 53
(71 4) (73 1000) (74 74) (86 6) (89 41)
(90 15) (91 6) (101 39) (103 29) (104 46)
(105 13) (131 20) (133 51) (145 4) (146 12)
(147 175) (148 18) (149 45) (150 4) (160 4)
(161 27) (162 5) (164 3) (173 7) (174 14)
(175 4) (176 3) (189 3) (191 29) (192 20)
(193 5) (205 8) (206 325) (207 73) (208 28)
(209 4) (219 5) (220 74) (221 83) (222 20)
(223 7) (233 6) (234 4) (235 15) (236 4)
(249 4) (264 6) (294 3) (308 4) (322 6)
(323 56) (324 16) (325 7)

NAME:13C_2028.6_1313EC11_
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:203002-11-1
RI:2029
RT:12.676
NUM PEAKS: 88
(70 33) (71 34) (72 236) (74 190) (75 1000)
(76 82) (77 52) (82 3) (83 29) (84 19)
(85 101) (86 45) (87 185) (88 114) (89 168)
(93 3) (96 3) (97 5) (98 35) (99 12)
(100 60) (102 213) (103 102) (104 101) (106 14)
(113 15) (114 6) (115 32) (116 38) (117 77)
(118 146) (119 527) (120 42) (121 20) (126 3)
(127 4) (128 22) (129 9) (130 32) (131 42)
(132 468) (134 188) (135 31) (136 8) (137 3)
(141 3) (142 4) (143 19) (144 20) (145 18)
(146 35) (148 164) (150 10) (157 3) (158 12)
(159 10) (160 23) (162 39) (163 47) (164 5)
(165 5) (175 15) (176 21) (177 28) (178 16)
(179 4) (181 3) (188 3) (189 6) (190 16)
(193 8) (194 4) (204 3) (237 6) (238 6)
(239 3) (250 3) (251 5) (252 29) (253 5)
(254 4) (301 3) (326 22) (327 106) (328 15)
(329 4) (341 3) (342 10)

NAME:13C_2039.3_1313EC11_
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:204003-11-1
RI:2039
RT:12.745
NUM PEAKS: 56
(73 1000) (74 83) (87 116) (101 75) (102 49)
(115 34) (130 113) (131 46) (133 47) (145 24)
(147 143) (149 20) (152 14) (159 23) (171 9)
(173 37) (175 313) (176 58) (177 53) (183 15)
(189 18) (190 18) (195 9) (203 57) (216 18)
(217 33) (218 346) (219 65) (222 10) (231 18)
(242 16) (262 16) (275 16) (277 17) (292 41)
(293 21) (345 15) (346 7) (378 17) (379 39)
(396 16) (425 12) (432 11) (438 8) (449 12)
(453 15) (462 14) (463 17) (473 16) (476 13)

(491 15) (508 17) (557 9) (566 14) (571 8)
(585 4)

NAME:13C_2048.0_1313EC11_Hexadecanoic acid (1TMS)
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:205001-11-1
RI:2048
RT:12.800
NUM PEAKS: 86
(70 8) (72 95) (73 1000) (74 227) (75 996)
(76 109) (77 53) (85 23) (86 10) (87 82)
(88 37) (89 108) (90 12) (91 15) (100 22)
(101 12) (102 76) (103 42) (104 65) (105 6)
(106 28) (107 3) (115 9) (118 161) (119 904)
(120 71) (121 35) (130 13) (132 489) (133 68)
(134 607) (135 85) (136 26) (137 3) (140 4)
(147 53) (148 223) (149 34) (150 11) (160 7)
(161 6) (162 16) (163 28) (164 11) (175 4)
(177 22) (178 9) (179 6) (192 32) (193 24)
(194 8) (206 4) (207 14) (208 50) (209 7)
(210 3) (211 3) (220 3) (222 10) (223 8)
(224 3) (233 3) (237 8) (238 11) (239 3)
(252 5) (253 11) (267 3) (268 6) (282 7)
(283 3) (284 6) (297 4) (298 12) (299 11)
(300 3) (315 4) (327 10) (328 38) (329 194)
(330 28) (331 7) (343 6) (344 21) (345 3)
(387 4)

NAME:13C_2087.2_1313EC11_
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:209004-11-1
RI:2087
RT:13.049
NUM PEAKS: 65
(71 8) (72 21) (73 1000) (74 86) (75 87)
(76 7) (85 9) (86 14) (87 10) (89 71)
(90 23) (91 7) (101 45) (102 15) (103 31)
(104 65) (105 16) (106 4) (114 5) (116 6)
(117 13) (118 16) (119 42) (131 23) (132 74)
(133 49) (134 12) (145 8) (146 17) (147 157)
(148 32) (149 50) (150 7) (160 8) (161 32)
(162 10) (163 9) (164 5) (173 10) (174 12)
(176 6) (187 3) (192 19) (193 4) (202 3)
(205 7) (206 362) (207 84) (208 30) (209 5)
(220 75) (221 92) (222 22) (223 7) (233 9)
(234 6) (235 18) (248 11) (249 4) (264 5)
(294 7) (322 9) (323 69) (324 20) (325 9)

NAME:13C_2063.4_1313EC11_
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:206001-11-1
RI:2063
RT:12.898
NUM PEAKS: 296
(70 45) (71 26) (72 65) (74 180) (75 213)
(79 27) (80 24) (81 33) (86 33) (87 255)
(89 32) (91 29) (95 34) (99 33) (100 24)
(101 131) (103 110) (105 33) (106 48) (109 37)
(112 26) (113 32) (114 36) (115 62) (116 33)
(117 99) (118 52) (119 205) (120 42) (122 42)

(125 21) (126 20) (128 33) (130 37) (131 72)
(132 33) (133 116) (135 31) (137 25) (139 26)
(140 51) (141 19) (142 25) (143 28) (144 40)
(145 42) (147 308) (148 107) (149 59) (150 23)
(151 45) (153 31) (157 31) (159 31) (160 60)
(161 48) (164 31) (165 42) (166 22) (167 21)
(168 24) (169 27) (171 23) (173 40) (174 56)
(175 1000) (176 223) (177 161) (178 42) (179 52)
(180 22) (182 29) (186 22) (188 25) (189 66)
(192 47) (201 49) (205 39) (206 23) (208 19)
(209 26) (210 22) (211 69) (212 60) (213 35)
(214 24) (215 39) (217 29) (219 31) (221 32)
(222 27) (224 41) (225 26) (226 30) (227 41)
(230 29) (231 37) (232 23) (233 28) (234 26)
(235 37) (236 47) (237 33) (239 21) (243 22)
(246 33) (247 59) (248 91) (249 29) (254 33)
(255 33) (256 33) (257 36) (261 20) (262 42)
(263 130) (264 46) (265 38) (266 41) (268 30)
(269 27) (271 26) (273 18) (274 43) (275 37)
(276 29) (277 20) (278 31) (279 37) (281 44)
(282 25) (289 22) (291 20) (292 36) (295 22)
(297 28) (299 63) (303 24) (305 34) (310 29)
(312 24) (313 42) (314 24) (315 61) (318 40)
(321 30) (322 21) (323 27) (324 48) (325 43)
(328 36) (329 35) (330 38) (332 30) (334 39)
(335 17) (337 38) (338 44) (340 26) (341 34)
(344 22) (346 18) (347 31) (350 23) (355 29)
(356 49) (357 27) (359 24) (360 24) (361 29)
(364 25) (365 29) (371 30) (374 38) (376 32)
(377 20) (383 20) (384 50) (385 50) (386 29)
(387 21) (388 28) (389 33) (390 29) (394 25)
(395 33) (397 35) (398 25) (399 29) (401 21)
(404 22) (405 26) (406 40) (407 31) (408 31)
(409 19) (411 24) (412 25) (414 32) (417 21)
(418 36) (419 22) (420 23) (422 31) (423 34)
(424 27) (425 26) (426 29) (427 29) (428 21)
(431 26) (432 23) (433 24) (434 32) (435 22)
(437 23) (438 30) (441 22) (442 29) (446 34)
(448 33) (449 16) (451 20) (453 31) (454 49)
(455 98) (456 50) (457 41) (459 21) (460 25)
(461 39) (462 37) (465 29) (466 25) (467 47)
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(480 25) (481 25) (482 38) (483 30) (485 27)
(487 27) (488 35) (492 30) (493 35) (494 28)
(495 34) (496 30) (498 26) (499 42) (500 25)
(501 44) (503 22) (504 36) (508 30) (509 26)
(510 36) (514 30) (515 23) (516 23) (517 35)
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(524 29) (526 25) (527 22) (528 37) (529 33)
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(538 26) (539 19) (542 30) (546 35) (547 52)
(550 24) (554 25) (560 18) (564 30) (565 15)
(566 21) (570 23) (571 21) (579 22) (583 14)
(592 14)

NAME:13C_2025.7_1313EC16_
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:203004-11-1
RI:2026
RT:12.686

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NUM PEAKS:   343
( 70   22) ( 71   55) ( 72   44) ( 73 1000) ( 74   58)
( 75  317) ( 76    5) ( 77   20) ( 78   11) ( 79   11)
( 80    8) ( 81    8) ( 82    4) ( 83   17) ( 84   38)
( 85   50) ( 86   29) ( 87   24) ( 88   17) ( 90    7)
( 92    9) ( 93    6) ( 94    3) ( 96    5) ( 97    7)
( 98   11) ( 99   20) (100   35) (101    5) (102   41)
(103   40) (104   11) (105   18) (106    9) (107   21)
(109    4) (111    4) (112    9) (113    3) (114   14)
(115   35) (116   27) (117   10) (118   17) (119   38)
(122   12) (123   15) (127   11) (129   10) (130    8)
(131   59) (132   79) (133   96) (135   18) (137   22)
(138    4) (141    9) (142    3) (143   10) (144    5)
(145   11) (146   20) (147  194) (148   46) (149   13)
(150    4) (151    9) (153   16) (154    6) (155   15)
(156   17) (157    8) (162   18) (164    4) (165   12)
(167   18) (169    5) (170    4) (171    3) (172   14)
(173   22) (174  155) (175   31) (176   12) (177    6)
(178    7) (179    3) (181   16) (182    4) (183   20)
(185    4) (187    7) (188   15) (189   43) (190    8)
(191    5) (192    3) (193   20) (194    7) (195    7)
(196    7) (197   10) (199    3) (200   10) (202    5)
(203    9) (204    3) (205    6) (210   10) (211  106)
(212   23) (213    3) (214   10) (215    3) (216   15)
(217    5) (218   15) (219   13) (223    4) (224    8)
(225   16) (226    9) (227   35) (228   13) (229    8)
(230    5) (231    3) (233    7) (234    6) (240    4)
(241   15) (242    4) (243   24) (244    6) (245    7)
(246    4) (247   69) (248  190) (249   54) (250   11)
(251   10) (252    8) (253    6) (254    9) (255   10)
(256   10) (257    8) (259    4) (260    3) (261    5)
(262   27) (263  134) (264   34) (265    8) (266    3)
(267   10) (268    6) (269    6) (273    4) (276    7)
(277    5) (278   11) (279   18) (280    5) (282   13)
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(291    8) (292    5) (293    7) (294    5) (295    3)
(296    6) (297    5) (298   14) (299  122) (300   56)
(301   19) (302    7) (303    9) (304    3) (307    6)
(308    5) (309    6) (313   13) (314   14) (315  101)
(316   29) (317   13) (320    3) (325   16) (326   19)
(327   21) (330    3) (332    3) (333    5) (334    9)
(335    3) (336   11) (337    9) (338    6) (341   12)
(342   16) (345    3) (346   13) (347    8) (348    6)
(349   11) (350    7) (352    9) (353    6) (354    3)
(355    6) (356   10) (357    8) (360    4) (361   14)
(362    7) (363    3) (364   18) (365   12) (366    3)
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(374    3) (376    4) (382    3) (383    3) (388    3)
(389   10) (391    3) (398    6) (399    6) (401    9)
(402    6) (403    5) (404    4) (405    3) (407    4)
(408    5) (409    4) (410    9) (411   15) (412    6)
(414    5) (415   10) (420    8) (421   11) (422    3)
(423    3) (427    6) (428    7) (430    7) (431   13)
(432   10) (433    9) (434    3) (436    6) (441    7)
(444    5) (445    3) (446    7) (452    7) (453    6)
(454    3) (455    7) (456    6) (457   10) (458    9)
(461    8) (462   14) (468    4) (469   11) (471    8)
(472    3) (473    7) (477    3) (478   11) (480    4)
(483    4) (484    6) (487    4) (488    5) (489    7)
(490    9) (491    8) (492    6) (494    7) (497   14)
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(501   10) (502   10) (504    4) (506    8) (507    5)
(508   11) (509    3) (510    3) (512    5) (513    4)
(514    4) (515    4) (519    8) (520    7) (522    5)
(527    6) (530    6) (532    7) (533   13) (535    5)
(537    4) (538    4) (539    3) (543    9) (544    8)
(545    4) (547    5) (550    5) (551    4) (552    7)
(553    3) (557    5) (558    7) (559    5) (560    6)
(566    4) (567    3) (568    5) (569    5) (571   10)
(572    5) (573    4) (574    3) (575    4) (580    6)
(581    5) (582    5) (597    3)

NAME:13C_2003.6_1313EC11_
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:200002-11-1
RI:2004
RT:12.518
NUM PEAKS:  114
( 72   48) ( 73  434) ( 74  140) ( 75  206) ( 76   23)
( 77   11) ( 86   16) ( 87  216) ( 88   32) ( 89   13)
( 94    5) ( 99   11) (100   68) (101  111) (102   42)
(103   22) (113   10) (114    7) (115   34) (116   31)
(117   50) (118   51) (123    5) (129   15) (130   72)
(131  114) (134    7) (135    7) (137    5) (143   27)
(144   16) (145   12) (146  126) (150    6) (152    4)
(156    9) (157   13) (158    7) (159   27) (160   50)
(163    4) (169    5) (173   28) (174   22) (175 1000)
(176  169) (177   78) (178    6) (184    4) (188    6)
(189   13) (190   15) (199    5) (200   20) (203   12)
(204    8) (205   44) (211    5) (215   11) (216    7)
(218   14) (219    7) (221   15) (230   10) (231  102)
(232   19) (233    6) (234   11) (235   10) (245    5)
(250    6) (259    6) (264   10) (265   21) (266    5)
(283    4) (284    6) (287    4) (288    5) (289    5)
(290    5) (291    9) (292    9) (297    6) (299    7)
(306    6) (316    7) (317    6) (320    6) (321   20)
(324   24) (325    6) (334    6) (335    5) (369    4)
(370    6) (380    4) (381    5) (382   18) (383    6)
(389    5) (396    5) (397    9) (418    5) (424    5)
(436    6) (443    4) (452    5) (456    5) (481    5)
(495    5) (534    6) (544    4) (548    5)

NAME:13C_1878.0_1313EC11_Fructose methoxyamine {BP} (5TMS)
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:188004-11-1
RI:1878
RT:11.688
NUM PEAKS:  68
( 70    5) ( 71    7) ( 72   20) ( 73 1000) ( 74   92)
( 75   79) ( 85   24) ( 86   13) ( 88    6) ( 89   55)
( 90   27) ( 91    4) (101    9) (102    9) (103   50)
(104  222) (105   34) (106    9) (114    3) (115    7)
(116   21) (117   10) (118   19) (119   59) (120    8)
(129    3) (130    3) (131   24) (132   70) (133   76)
(135   12) (145    8) (146   14) (147  217) (148   52)
(164    3) (175    3) (176   11) (177    8) (178    3)
(190    4) (191   32) (192   24) (193    6) (203    7)
(204    6) (208   17) (219   11) (220  172) (221   40)
(222   18) (235    7) (236    3) (248    6) (249    3)
(262    4) (265    8) (266    5) (279   10) (280    4)
(294    3) (308    3) (309    5) (310   40) (311   11)
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(312 5) (338 4) (368 6)

NAME:13C_1824.4_1313EC11_
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:182006-11-1
RI:1824
RT:11.274
NUM PEAKS: 205

(76 309)	(77 511)	(78 165)	(79 428)	(81 43)
(82 42)	(83 61)	(84 208)	(91 135)	(92 44)
(93 247)	(94 42)	(95 133)	(96 59)	(97 112)
(107 30)	(108 23)	(109 22)	(110 35)	(111 51)
(112 42)	(120 31)	(121 32)	(124 13)	(125 41)
(126 58)	(127 78)	(137 24)	(140 38)	(141 87)
(142 52)	(152 37)	(153 27)	(154 25)	(155 57)
(156 34)	(165 30)	(169 62)	(170 124)	(182 23)
(184 117)	(195 28)	(196 48)	(197 73)	(198 118)
(199 35)	(200 20)	(210 49)	(212 106)	(214 31)
(224 27)	(225 25)	(226 26)	(227 27)	(228 29)
(240 27)	(241 33)	(242 49)	(243 36)	(244 22)
(245 43)	(254 35)	(255 23)	(256 26)	(268 25)
(269 204)	(270 1000)	(271 209)	(272 97)	(282 21)
(283 27)	(284 98)	(285 353)	(286 82)	(287 34)
(288 10)	(296 10)	(297 8)	(298 19)	(299 75)
(300 19)	(302 22)	(304 25)	(310 60)	(311 38)
(312 26)	(313 22)	(314 32)	(315 30)	(316 19)
(317 16)	(324 24)	(325 30)	(326 14)	(327 21)
(328 27)	(329 12)	(330 21)	(331 26)	(332 19)
(333 35)	(340 10)	(341 9)	(342 12)	(345 15)
(346 23)	(356 10)	(359 9)	(362 24)	(366 29)
(371 13)	(372 11)	(378 12)	(387 18)	(388 7)
(391 10)	(394 13)	(395 14)	(396 15)	(397 21)
(398 25)	(399 16)	(400 17)	(401 15)	(404 20)
(405 20)	(406 10)	(414 17)	(415 19)	(416 15)
(417 16)	(418 18)	(419 17)	(420 23)	(421 15)
(422 22)	(430 11)	(431 14)	(432 12)	(434 14)
(435 12)	(436 10)	(437 13)	(438 24)	(439 18)
(440 19)	(441 9)	(442 13)	(443 18)	(444 21)
(445 9)	(452 10)	(453 10)	(454 11)	(456 12)
(464 26)	(466 28)	(467 17)	(468 11)	(469 16)
(474 20)	(475 13)	(489 9)	(492 12)	(493 14)
(494 14)	(495 17)	(496 8)	(497 13)	(501 12)
(505 8)	(506 8)	(509 12)	(511 18)	(512 21)
(513 17)	(514 13)	(516 16)	(517 13)	(518 19)
(520 12)	(521 9)	(522 23)	(523 12)	(524 13)
(525 12)	(526 20)	(527 17)	(528 19)	(529 9)
(530 11)	(531 14)	(536 8)	(538 11)	(540 10)
(541 18)	(542 14)	(543 8)	(546 13)	(548 15)
(552 7)	(556 4)	(561 8)	(588 4)	(592 4)

NAME:13C_1822.9_1313EC11_Citric acid (4TMS)
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:182004-11-1
RI:1823
RT:11.261
NUM PEAKS: 145

(70 24)	(71 111)	(72 59)	(73 1000)	(74 10)
(75 352)	(76 22)	(77 29)	(78 3)	(79 5)
(83 4)	(84 9)	(85 24)	(89 4)	(93 12)
(95 8)	(96 5)	(97 9)	(98 5)	(99 21)

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(100    8) (105    8) (111    5) (118   13) (119   10)
(127    3) (129   10) (132    8) (133  110) (134   10)
(135   12) (139    4) (141    9) (142    3) (143   15)
(147  526) (148   33) (149  126) (150   16) (151   10)
(155    3) (161    4) (163   13) (169    5) (170    5)
(171    4) (183   28) (184    8) (185   11) (187    5)
(188   75) (189   16) (190    9) (191    6) (193    4)
(197    3) (198    4) (201    3) (207   19) (208    4)
(209    3) (211   41) (212    9) (213    7) (215    8)
(216   10) (217  112) (219   10) (221   63) (222   12)
(223    8) (229    5) (231    7) (232    4) (233   12)
(234   10) (235   13) (245    3) (257   18) (258    4)
(259    4) (261   11) (262   51) (269    8) (270   43)
(271    8) (272    7) (273  136) (274   31) (275   14)
(276    7) (277   33) (278  378) (279   68) (280   32)
(281    4) (284    4) (285   19) (286    4) (287    3)
(291   13) (292    3) (293    6) (299    3) (301    3)
(303    4) (305    9) (306    5) (307   16) (308   23)
(309    9) (310    5) (323    5) (337    3) (338    3)
(346    3) (347   26) (348    9) (349    5) (350    3)
(351   15) (352   80) (353   23) (354   11) (363   18)
(364    6) (365    3) (367    9) (368   55) (369   16)
(370    7) (374    3) (375   20) (376    6) (377    3)
(380   11) (381   56) (382   17) (383    9) (465    8)
(466    3) (470    7) (471   24) (472   10) (473    3)

NAME:13C_1741.3_1313EC11_
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:174003-11-1
RI:1741
RT:10.629
NUM PEAKS:  33
( 72   33) ( 73 1000) ( 74   59) ( 75   97) ( 76   13)
(101  106) (108   11) (113   16) (116   14) (117   22)
(129   19) (130   21) (131   44) (133   48) (143   17)
(147  280) (148   42) (149   22) (163   99) (173   82)
(174   20) (184   10) (204   48) (205   44) (207  215)
(208   29) (221   14) (231   48) (281   17) (291    9)
(292   21) (307   29) (410   12)

NAME:13C_1694.3_1313EC11_
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:169001-11-1
RI:1694
RT:10.264
NUM PEAKS:  44
( 70   12) ( 73 1000) ( 74   53) ( 75   61) ( 90   60)
( 93   10) (103   86) (104   53) (107   14) (114   14)
(117   46) (119  183) (131   23) (132   55) (133   91)
(134   11) (135   16) (147  207) (148   37) (149   26)
(153    8) (155   11) (158   12) (191   20) (219   46)
(220   22) (235   41) (236   19) (245    8) (249    9)
(250   39) (254   16) (264   29) (271   16) (292   16)
(313    9) (323   16) (346   21) (347   13) (358   13)
(392   15) (405   14) (458   12) (459   10)

NAME:13C_1673.0_1313EC07_
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:167003-11-1
RI:1673
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RT:10.101
NUM PEAKS:  60
( 73 1000) ( 74  100) ( 75  212) ( 76   15) ( 85   14)
( 86   50) ( 87  123) ( 98    3) ( 99    8) (100   11)
(102   55) (103  476) (112    4) (115   29) (117   17)
(118   27) (127    3) (142    3) (144    7) (158   11)
(159    7) (160   39) (161   26) (172    3) (175   51)
(176   28) (184    2) (186    3) (187    2) (188    4)
(189   18) (200    2) (201    2) (204    5) (214    2)
(215    2) (229    2) (230    2) (248   11) (249    9)
(250    5) (277    3) (292    6) (293   69) (294  500)
(295   99) (296   43) (297    5) (321    2) (322    8)
(323    3) (350    2) (351   10) (352    4) (353    3)
(368   13) (369    5) (370    2) (396    2) (397    2)

NAME:13C_1562.0_1313EC11_Cysteine (3TMS)
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:156002-11-1
RI:1562
RT:9.232
NUM PEAKS:  115
( 70  174) ( 71  121) ( 72   45) ( 73 1000) ( 74  199)
( 75  502) ( 76   45) ( 77   24) ( 80    9) ( 81    9)
( 82   17) ( 83  124) ( 85  100) ( 86   14) ( 87   44)
( 88   37) ( 89   41) ( 90    9) ( 91   49) ( 92    8)
( 94    5) ( 95    5) ( 96   35) ( 97   41) ( 98  351)
( 99   49) (100   68) (101   60) (102   39) (103   30)
(104   55) (105    4) (106    6) (110   24) (111  140)
(112   13) (113   17) (114    9) (115   13) (116    8)
(117   23) (118   35) (119   31) (120    6) (121    4)
(123    3) (124    6) (125   23) (126   63) (127  144)
(130    5) (131   23) (132  250) (133   72) (134   26)
(135    5) (137    3) (139   26) (140    8) (141    9)
(143   12) (145    6) (146    5) (147  130) (153    5)
(154    5) (155    9) (156   13) (157    6) (158    6)
(159   67) (161   12) (163    8) (168    9) (169   10)
(172    6) (173    9) (174    4) (175   14) (177    5)
(183    6) (184   15) (185   21) (187    4) (200    3)
(201    4) (202   18) (206    8) (208    4) (212    4)
(213   42) (214    8) (218    5) (219    5) (220   76)
(221   19) (222   81) (223   13) (224   10) (230    5)
(231   30) (232    4) (235    5) (236    3) (237    8)
(244    4) (250    3) (251    9) (252    4) (264    4)
(265    3) (279    3) (285    5) (286    3) (296    4)

NAME:13C_1279.2_1313EC16_Serine (2TMS)
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:128001-11-1
RI:1279
RT:6.160
NUM PEAKS:  40
( 72   20) ( 73 1000) ( 74  114) ( 75  320) ( 76   27)
( 77    9) ( 81   44) ( 86    7) ( 87   86) ( 88   32)
( 89   41) ( 90    9) ( 91    7) (101   40) (102   91)
(103   27) (104  112) (105    8) (116   28) (117   39)
(118  652) (119   67) (120   20) (130    5) (131   14)
(132   60) (133   82) (134  446) (135   36) (136   12)
(145    6) (147   89) (148   54) (149   12) (162   30)
(174    5) (208    5) (221   20) (228    7) (237   17)
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NAME:13C_1220.5_1313EC11_Valine (2TMS)
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:122001-11-1
RI:1221
RT:5.509
NUM PEAKS:  25
( 70    12) ( 72    35) ( 73   981) ( 74   127) ( 75   355)
( 76    99) ( 79    48) ( 87    43) ( 88    19) (100    21)
(101   112) (102    28) (103    16) (104    13) (117    35)
(131    23) (132    66) (133    58) (147   192) (148 1000)
(149   100) (150    39) (161    15) (220    75) (222    41)

NAME:13C_1314.0_1313EC16_Isoleucine (2TMS)
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:132002-11-1
RI:1314
RT:6.570
NUM PEAKS:  27
( 90     6) ( 91    25) (101    80) (118     8) (132    49)
(158    10) (160     9) (161     9) (162    47) (163 1000)
(164    88) (165    30) (196     1) (203     1) (204     2)
(205     6) (207     5) (215     1) (220    52) (236     2)
(237    37) (238     9) (239     3) (266     8) (267     2)
(268     1) (347     1)

NAME:13C_1354.8_1313EC11_Glyceric acid (3TMS)
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:135003-11-1
RI:1355
RT:7.049
NUM PEAKS:  14
( 73 1000) ( 74    82) (103   176) (104   107) (118    23)
(119    71) (131    35) (132    50) (133   190) (147   359)
(148    57) (191   224) (207    37) (294    62)

NAME:13C_1372.0_1313EC11_Fumaric acid (2TMS)
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:137001-11-1
RI:1372
RT:7.282
NUM PEAKS:  124
( 70    21) ( 71    81) ( 72     7) ( 73 1000) ( 74   112)
( 75   527) ( 76    32) ( 80     9) ( 81    21) ( 82    27)
( 83   114) ( 84    43) ( 85   152) ( 86    42) ( 94    12)
( 95    11) ( 97    17) ( 98     5) (101    15) (103     9)
(104     3) (105    14) (106     4) (108    10) (109     8)
(110    16) (111     7) (112    17) (113     5) (114     6)
(115    68) (116    21) (117    56) (118     9) (119     4)
(124     7) (127    27) (128    13) (129    24) (130    19)
(131    28) (132     8) (133   137) (134    25) (135    16)
(136     4) (139    10) (141     4) (142     6) (143   111)
(144    25) (145    22) (146    90) (147   792) (148   127)
(149    90) (150    17) (151     4) (152    14) (155    43)
(156    24) (157    40) (158    15) (159    56) (160     1)
(165     3) (167     3) (170     4) (171    41) (172    16)
(176     1) (177    12) (178     6) (180     2) (185     1)
(186     2) (188     3) (190     3) (191    12) (192     7)
(193     2) (195     9) (198     1) (199    12) (200     3)
(202     8) (206     1) (209     4) (210     6) (214     2)
(216     2) (217    22) (218    11) (219     5) (220    15)
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(221 8) (225 7) (228 3) (229 2) (230 4)
(231 3) (232 1) (234 6) (238 3) (240 6)
(244 12) (245 437) (246 91) (247 32) (248 28)
(249 324) (250 48) (251 15) (253 2) (254 6)
(259 2) (260 4) (264 1) (265 3) (269 10)
(270 6) (271 12) (272 2) (273 2)

NAME:13C_1449.3_1313EC16_
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:144007-11-1
RI:1449
RT:8.163
NUM PEAKS: 308
(72 69) (73 1000) (74 220) (75 423) (76 73)
(77 47) (79 38) (82 2) (83 12) (84 4)
(85 17) (86 16) (87 9) (88 15) (89 27)
(90 16) (91 12) (92 25) (93 9) (94 8)
(97 6) (98 19) (100 19) (101 47) (102 65)
(103 41) (104 50) (105 18) (109 14) (110 7)
(111 10) (112 11) (115 32) (116 11) (117 23)
(118 202) (119 154) (120 14) (121 21) (122 16)
(126 3) (128 8) (129 5) (130 14) (131 23)
(132 207) (133 73) (134 9) (135 12) (137 11)
(138 12) (139 1) (140 15) (142 32) (143 4)
(146 21) (147 328) (148 57) (149 35) (151 8)
(152 2) (155 10) (156 29) (158 15) (159 15)
(160 15) (162 27) (163 327) (164 27) (165 10)
(167 2) (168 5) (169 3) (171 1) (174 6)
(175 22) (176 14) (177 2) (179 4) (180 10)
(181 7) (182 11) (184 9) (186 27) (187 9)
(190 2) (192 1) (193 12) (195 15) (196 5)
(197 17) (200 27) (201 3) (202 22) (204 13)
(205 25) (206 1) (207 9) (212 8) (214 8)
(216 6) (223 6) (226 18) (229 7) (232 5)
(234 13) (235 13) (236 25) (237 17) (238 1)
(241 2) (242 5) (246 4) (249 42) (250 1)
(252 17) (255 11) (256 2) (257 19) (258 27)
(259 2) (266 12) (269 5) (272 6) (276 19)
(277 3) (278 9) (281 1) (283 24) (284 8)
(288 6) (289 2) (290 7) (294 7) (295 3)
(298 4) (312 13) (313 1) (314 7) (315 1)
(321 5) (322 4) (326 7) (327 18) (328 7)
(329 6) (330 2) (333 7) (334 18) (335 17)
(336 8) (337 3) (338 4) (342 18) (344 9)
(345 18) (346 5) (349 13) (350 5) (352 6)
(353 7) (354 12) (356 20) (357 11) (358 21)
(361 15) (362 14) (363 6) (365 8) (366 19)
(367 9) (368 18) (370 1) (371 2) (372 5)
(373 11) (375 16) (379 6) (380 6) (381 22)
(382 2) (383 18) (384 8) (386 11) (387 3)
(388 7) (389 18) (390 10) (393 8) (394 6)
(396 10) (397 8) (400 22) (401 2) (402 18)
(404 11) (405 10) (406 4) (407 7) (409 11)
(410 1) (413 1) (414 21) (415 5) (416 26)
(417 13) (419 2) (422 5) (424 9) (425 1)
(426 15) (429 10) (431 12) (432 8) (433 10)
(436 13) (438 23) (441 8) (444 27) (445 8)
(447 3) (448 6) (449 12) (452 18) (453 15)
(454 11) (457 13) (459 4) (460 24) (461 16)
(462 1) (464 8) (466 18) (467 5) (471 12)

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(472   15) (475   31) (476    3) (477    1) (481   10)
(482   13) (483    2) (486    2) (487    3) (488   14)
(489   29) (490   21) (492    1) (493    3) (494   18)
(496    3) (499   17) (500    7) (502    6) (503    3)
(506   24) (507    9) (508    1) (509   28) (511   12)
(512    6) (513    3) (517   11) (518   14) (519    1)
(523   12) (525   14) (527   12) (530   23) (531   19)
(533    4) (534   14) (535    2) (537    9) (538    6)
(539    4) (541   15) (542    5) (548   12) (553   13)
(554    5) (559    3) (560    4) (563   14) (564    3)
(565    7) (568    2) (569   11) (571   11) (573    3)
(574    4) (575   12) (576    4) (578    4) (579    4)
(580    5) (582    6) (583    9) (584    1) (585    1)
(586    1) (587    6) (591    1) (592   17) (593    4)
(595    3) (596    3) (597    1)

NAME:13C_1726.4_1313EC11_Fucose methoxyamine (4TMS)
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:173002-11-1
RI:1726
RT:10.512
NUM PEAKS:  37
( 72  106) ( 73  999) (103  153) (106   69) (116   32)
(117   68) (118   45) (119 1000) (120   73) (131  164)
(134   51) (135   40) (137   33) (146   50) (148  204)
(149  120) (175   25) (190   63) (191  164) (192  128)
(193   40) (205   27) (219   34) (222   65) (235   26)
(249   25) (250  123) (260   14) (294   32) (309   19)
(311   36) (322   52) (324   40) (337   33) (398   20)
(500   17) (537   15)

NAME:13C_1785.2_1313EC07_
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:179001-11-1
RI:1785
RT:10.978
NUM PEAKS:  337
( 72   18) ( 73 1000) ( 74   72) ( 75   49) ( 76    9)
( 78    3) ( 82    3) ( 86    3) ( 88    3) ( 89    5)
( 90   18) ( 91   12) ( 92    2) ( 94    2) ( 96    1)
( 97    2) (103   52) (104  225) (105   24) (106    9)
(107    2) (108    2) (109    2) (115    8) (117    3)
(118    9) (119   58) (120    6) (121    4) (122    2)
(128    1) (129    3) (131   21) (132   63) (133   93)
(134   29) (135   13) (138    2) (140    2) (141    1)
(144    2) (145    9) (146   29) (147  213) (148   42)
(149   34) (150    7) (151    4) (152    1) (154    1)
(155    3) (157    1) (159    2) (161   10) (162    3)
(163    2) (164    3) (165    4) (166    1) (167    3)
(168    2) (176    3) (177    8) (178    3) (179    4)
(180    3) (181    6) (182    2) (183    2) (184    2)
(187    1) (188    2) (189    4) (191   47) (192   22)
(193    9) (195    7) (196    1) (197    2) (199    2)
(200    2) (202    1) (205    4) (206   51) (207   41)
(208    9) (209    4) (210    4) (211   12) (213    3)
(214    2) (215    1) (216    1) (217    2) (218    2)
(219    5) (220  131) (221   42) (222   15) (223    3)
(224    1) (228    3) (231    1) (233    3) (234    3)
(238    1) (239    2) (240    1) (242    3) (243    3)
(244    2) (245    2) (246    1) (247    1) (248    1)
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(249 3)	(252 2)	(253 2)	(254 2)	(256 3)
(257 2)	(259 3)	(261 1)	(262 9)	(263 4)
(264 5)	(266 3)	(269 2)	(272 1)	(273 1)
(274 2)	(275 2)	(276 2)	(277 2)	(279 14)
(280 5)	(281 1)	(282 2)	(284 1)	(285 4)
(286 2)	(287 2)	(288 1)	(291 1)	(292 3)
(293 11)	(294 137)	(295 38)	(296 18)	(297 3)
(298 4)	(299 6)	(300 4)	(301 4)	(302 2)
(303 1)	(305 1)	(306 1)	(307 5)	(308 20)
(309 8)	(310 19)	(311 5)	(312 3)	(315 3)
(316 2)	(317 2)	(318 2)	(319 2)	(320 1)
(322 1)	(323 3)	(324 3)	(330 2)	(332 3)
(333 2)	(335 3)	(336 10)	(337 15)	(338 6)
(339 3)	(340 2)	(343 1)	(345 2)	(346 2)
(348 2)	(349 3)	(351 6)	(352 5)	(353 3)
(354 1)	(358 2)	(360 2)	(362 2)	(363 2)
(364 2)	(365 1)	(366 2)	(369 2)	(370 1)
(372 3)	(373 4)	(374 3)	(375 2)	(382 3)
(383 2)	(384 2)	(386 2)	(387 3)	(389 2)
(390 3)	(391 2)	(392 2)	(394 2)	(396 2)
(397 2)	(398 1)	(399 2)	(400 1)	(404 2)
(405 2)	(406 2)	(408 2)	(410 1)	(411 1)
(412 1)	(416 2)	(420 1)	(421 2)	(422 2)
(423 2)	(424 3)	(425 2)	(426 5)	(427 3)
(428 1)	(432 2)	(433 2)	(434 2)	(435 3)
(436 2)	(438 2)	(439 2)	(440 1)	(441 2)
(442 2)	(444 2)	(445 3)	(446 2)	(447 2)
(448 3)	(449 2)	(450 2)	(451 1)	(452 2)
(453 2)	(454 2)	(455 1)	(456 2)	(457 2)
(458 1)	(459 1)	(460 2)	(461 2)	(462 2)
(463 2)	(464 2)	(465 3)	(467 1)	(468 1)
(469 1)	(470 2)	(472 2)	(473 2)	(474 2)
(475 1)	(478 2)	(480 2)	(481 2)	(483 2)
(485 2)	(486 2)	(487 2)	(488 2)	(489 1)
(490 2)	(491 2)	(492 1)	(496 1)	(497 1)
(498 2)	(499 2)	(500 2)	(502 2)	(503 1)
(504 2)	(506 1)	(508 2)	(510 1)	(511 2)
(512 2)	(513 1)	(514 2)	(515 3)	(516 4)
(517 3)	(518 2)	(519 2)	(520 2)	(521 1)
(522 2)	(523 2)	(525 3)	(526 2)	(527 2)
(530 2)	(531 1)	(533 2)	(534 2)	(535 2)
(539 2)	(540 2)	(541 3)	(544 1)	(545 2)
(546 1)	(548 1)	(552 2)	(555 1)	(556 1)
(559 1)	(564 1)	(570 1)	(571 1)	(572 1)
(573 1)	(575 1)			

NAME:13C_1802.7_1313EC07_
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:180002-11-1
RI:1803
RT:11.114
NUM PEAKS: 85

(72 9)	(73 1000)	(74 103)	(75 108)	(76 12)
(87 5)	(90 8)	(92 1)	(94 1)	(102 4)
(103 21)	(104 13)	(114 5)	(116 2)	(118 9)
(119 25)	(130 1)	(131 27)	(132 46)	(133 32)
(134 6)	(135 7)	(136 1)	(140 4)	(144 2)
(145 26)	(146 21)	(147 102)	(148 15)	(149 11)
(157 2)	(159 1)	(161 19)	(174 9)	(177 1)
(186 1)	(188 2)	(189 2)	(190 1)	(191 15)

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(192   35) (193    8) (194    3) (207    9) (208    2)
(218    2) (219   10) (220   34) (221   24) (233    6)
(234    3) (242    1) (248    2) (249    1) (250    3)
(251    4) (252    1) (260    1) (261    2) (262   49)
(263    6) (264    3) (278    6) (279    4) (292    1)
(294    3) (295   12) (296    1) (297    1) (307    6)
(308    1) (323    6) (324    1) (352    5) (353    2)
(354    2) (368    2) (369    1) (429    1) (441    7)
(442   30) (443   14) (444    5) (512    1) (564    1)

NAME:13C_1805.7_1313EC07_
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:181004-11-1
RI:1806
RT:11.136
NUM PEAKS:  125
( 70   10) ( 71    8) ( 72   12) ( 73 1000) ( 74  100)
( 75  144) ( 76   13) ( 77    8) ( 81    3) ( 82    5)
( 83   16) ( 84    5) ( 85    5) ( 86   11) ( 87    5)
( 90   10) ( 91    5) ( 92    1) ( 93    1) ( 94    1)
( 95    2) ( 96    3) ( 97   15) ( 98    3) (100    2)
(101    3) (102    4) (103   17) (104   28) (109    1)
(110    1) (111    7) (112    2) (114    6) (115    3)
(116    5) (117    5) (118   10) (119   41) (120    3)
(121    1) (124    2) (125    3) (129    7) (130    2)
(131   22) (132   50) (133   34) (134    7) (135    6)
(136    1) (140    5) (141    1) (144    3) (145   27)
(146   15) (147  110) (148   18) (149   22) (150    2)
(151    1) (152    2) (153    1) (154    1) (159    1)
(160    4) (161   19) (174   15) (176    2) (179    1)
(188    3) (189    2) (190    2) (191   13) (196    2)
(201    2) (204    3) (214    1) (217    2) (218    5)
(219   15) (220   98) (221   34) (222    8) (223    2)
(224    1) (233    7) (234    6) (237    1) (248    3)
(249    1) (251    3) (260    1) (261    4) (262   56)
(263    8) (264    5) (265    2) (276    1) (278    4)
(279    4) (280    1) (294    2) (295    8) (296    2)
(307    8) (308    3) (309    1) (317    2) (323    7)
(324    2) (336    1) (351    1) (352    7) (353    2)
(354    2) (368    3) (369    1) (370    1) (440    1)
(441   10) (442   40) (443   17) (444    8) (445    1)

NAME:13C_1842.0_1313EC11_
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:184002-11-1
RI:1842
RT:11.427
NUM PEAKS:  140
( 70   11) ( 71    8) ( 72   30) ( 73 1000) ( 74  101)
( 75  178) ( 76   10) ( 77   17) ( 78    3) ( 79    4)
( 85   75) ( 86    6) ( 87   19) ( 88    5) ( 89    6)
( 90   15) ( 91    3) ( 92    1) ( 93    4) ( 94    1)
( 95    3) ( 97    1) ( 98    6) ( 99   25) (100   23)
(101   28) (102   16) (103   55) (104   44) (105    9)
(106    2) (113    3) (114    9) (115   13) (116    8)
(117   15) (118   16) (119   72) (120    5) (121    1)
(127    1) (129   10) (130   10) (131   23) (133   56)
(134   12) (135    4) (141   11) (142    6) (143    8)
(144    5) (145   16) (146   13) (147  171) (148   29)
(157   31) (158   28) (159   10) (160    4) (161    7)
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(162   14) (163    1) (170    4) (171   19) (172   72)
(173  526) (174  227) (175   32) (176    6) (177    6)
(178    2) (179    1) (185    3) (186    3) (187    7)
(188    2) (189    2) (190    2) (191    5) (192   15)
(193    3) (198    1) (199    1) (200    1) (201   13)
(202    3) (203    2) (204    1) (209    1) (211    1)
(212    1) (213    5) (214    1) (215    2) (216    1)
(217    1) (219    2) (220   19) (221    5) (222    3)
(231    2) (232    2) (243    6) (244    9) (245   25)
(246   29) (247    8) (248    1) (260    3) (261    5)
(262   23) (263    5) (264    1) (266    3) (270    3)
(273    1) (274    1) (275    8) (276    3) (285    1)
(289    1) (290   13) (291    3) (307    3) (308    1)
(334    6) (335    2) (336    2) (337    1) (352    2)
(353    1) (365    5) (366    1) (374    1) (380    9)
(381    2) (441    3) (442   15) (443    6) (444    1)

NAME:13C_1847.4_1313EC07_
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:185003-11-1
RI:1847
RT:11.461
NUM PEAKS:  205
( 71  111) ( 74  923) ( 75  999) ( 76   60) ( 77   33)
( 80    5) ( 86   69) ( 87  109) ( 88   35) ( 89  133)
( 90  149) ( 91   23) ( 92    9) ( 94    6) ( 96   11)
(101  170) (102  109) (104  542) (105   78) (106   25)
(108    5) (112   16) (115  158) (116   59) (118  157)
(120   49) (121   25) (130   87) (131  346) (132  605)
(134  142) (135   76) (136   10) (138    6) (139    5)
(144   76) (146  151) (150   38) (151   22) (153    4)
(155   15) (159   84) (160 1000) (161  714) (162  190)
(163  178) (164   33) (165   11) (166    5) (167    3)
(168    4) (178   44) (179   14) (184    7) (188   14)
(189   37) (190   27) (191  374) (196    3) (197    7)
(198   11) (203   40) (204   47) (205   61) (207  249)
(209   23) (210    4) (212    8) (215   10) (217   22)
(218   40) (223   30) (224    8) (226    4) (229    7)
(230   13) (232   73) (233   49) (234   99) (235   97)
(236   35) (237   22) (238    9) (239    4) (248  150)
(249   72) (250   32) (251   60) (252   12) (253    7)
(254    4) (256    3) (261   12) (263   18) (269    8)
(271    4) (272    5) (274   14) (277   58) (278   29)
(280   10) (281   10) (282    5) (289   13) (292   10)
(294   35) (295   12) (296    5) (297    3) (298    5)
(306   16) (307   22) (319    5) (321   21) (322  271)
(323  212) (324   81) (325   22) (326    8) (331    5)
(335   20) (338   14) (339    6) (340    4) (341    6)
(342    5) (343    4) (346    5) (347    6) (348    5)
(349    7) (350   11) (351   55) (352   46) (353   22)
(354   11) (359    4) (362    6) (363    3) (368   11)
(369    6) (372    6) (377    4) (383    5) (384    5)
(387    4) (388    5) (391    5) (396    8) (397    8)
(398    8) (404    3) (405    6) (410    3) (412    9)
(413    5) (416    4) (424    7) (425   33) (426   13)
(427    6) (431    3) (434    3) (438    5) (439    6)
(440    4) (441   10) (444   10) (447    6) (448    5)
(454    4) (455    3) (459    4) (461    5) (462    5)
(463    4) (466    7) (467    5) (469    4) (470    4)
(477    5) (489    3) (492    2) (496    5) (499    3)
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(504 4)	(521 3)	(527 4)	(538 2)	(541 3)
(542 4)	(545 3)	(551 2)	(553 3)	(556 2)
(559 2)	(560 3)	(563 3)	(567 2)	(569 4)
(570 2)	(572 4)	(573 2)	(588 3)	(590 2)

NAME:13C_1869.1_1313EC11_Fructose methoxyamine (5TMS)
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:187002-11-1
RI:1869
RT:11.620
NUM PEAKS: 110

(72 19)	(73 1000)	(74 96)	(76 3)	(85 19)
(86 5)	(88 5)	(89 19)	(90 19)	(91 3)
(92 1)	(102 6)	(103 35)	(104 174)	(105 20)
(106 7)	(107 1)	(116 9)	(117 9)	(118 7)
(119 50)	(120 5)	(121 2)	(131 26)	(132 25)
(133 55)	(134 23)	(135 8)	(136 1)	(145 7)
(146 7)	(147 206)	(148 38)	(149 23)	(150 2)
(151 1)	(160 4)	(161 5)	(163 4)	(164 2)
(165 1)	(175 2)	(176 9)	(177 8)	(178 4)
(179 1)	(188 2)	(190 2)	(191 15)	(192 8)
(193 3)	(194 1)	(203 6)	(204 3)	(205 3)
(206 16)	(207 18)	(208 5)	(209 2)	(210 1)
(217 4)	(218 2)	(219 5)	(220 80)	(221 17)
(222 8)	(223 1)	(233 2)	(234 2)	(235 1)
(236 1)	(237 1)	(249 1)	(250 1)	(261 2)
(262 1)	(263 1)	(264 1)	(265 2)	(266 3)
(267 1)	(268 1)	(277 1)	(278 1)	(279 7)
(280 3)	(281 2)	(282 1)	(291 1)	(293 1)
(294 2)	(295 1)	(296 1)	(305 1)	(306 1)
(307 1)	(308 1)	(309 2)	(310 28)	(311 7)
(312 3)	(335 1)	(337 1)	(338 2)	(339 1)
(354 1)	(367 1)	(368 4)	(369 2)	(370 1)

NAME:13C_2137.1_1313EC16_
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:214003-11-1
RI:2137
RT:13.366
NUM PEAKS: 65

(72 12)	(73 1000)	(74 81)	(75 68)	(85 12)
(86 11)	(87 15)	(89 32)	(90 19)	(99 6)
(101 4)	(102 10)	(103 21)	(104 181)	(105 15)
(106 7)	(116 15)	(117 10)	(118 10)	(119 67)
(120 4)	(131 25)	(132 77)	(133 50)	(134 46)
(135 7)	(145 4)	(146 12)	(147 244)	(148 35)
(149 18)	(151 5)	(158 6)	(161 67)	(162 7)
(169 3)	(173 19)	(174 5)	(176 8)	(177 8)
(191 25)	(192 11)	(203 6)	(204 5)	(206 28)
(207 120)	(208 20)	(220 74)	(233 14)	(235 8)
(236 3)	(250 4)	(265 6)	(274 3)	(279 7)
(308 4)	(322 12)	(323 118)	(324 35)	(325 14)
(422 4)	(449 3)	(466 5)	(478 3)	(590 3)

NAME:13C_2246.0_1313EC16_Octadecanoic acid (1TMS)
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:225002-11-1
RI:2246
RT:14.010
NUM PEAKS: 87

(72 70) (75 1000) (76 106) (77 52) (78 7)
(88 25) (89 82) (90 9) (91 31) (92 9)
(93 17) (94 3) (106 20) (107 10) (118 135)
(119 540) (120 41) (121 30) (125 3) (128 7)
(132 504) (134 364) (135 69) (136 17) (146 22)
(148 153) (149 31) (151 6) (158 4) (160 7)
(162 12) (163 23) (170 3) (178 3) (187 12)
(192 20) (194 4) (205 3) (208 35) (214 4)
(219 4) (220 12) (223 9) (233 4) (234 5)
(235 5) (237 6) (246 5) (252 7) (253 8)
(254 3) (260 3) (265 4) (268 13) (269 3)
(279 3) (284 3) (308 3) (313 6) (314 7)
(319 4) (323 4) (328 6) (334 3) (337 4)
(357 15) (358 28) (359 97) (360 19) (367 3)
(374 18) (395 3) (400 5) (421 4) (427 3)
(434 3) (436 3) (443 3) (444 5) (467 4)
(488 3) (491 4) (499 5) (506 4) (507 4)
(520 3) (535 3)

NAME:13C_2327.6_1313EC16_Glucose-6-phosphate methoxyamine (6TMS)
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:233002-11-1
RI:2328
RT:14.442
NUM PEAKS: 51
(72 20) (73 1000) (74 79) (75 77) (80 17)
(87 19) (89 36) (101 18) (103 46) (104 30)
(105 39) (116 21) (118 25) (119 18) (131 30)
(132 72) (133 77) (134 24) (135 29) (142 10)
(146 20) (147 150) (148 24) (161 50) (162 85)
(175 12) (191 14) (193 18) (206 17) (207 20)
(211 37) (220 32) (225 20) (260 7) (275 9)
(278 14) (283 12) (299 100) (300 30) (314 15)
(315 41) (317 12) (332 13) (359 36) (360 18)
(386 32) (387 113) (388 46) (389 25) (476 10)
(541 11)

NAME:13C_2748.0_1313EC16_Trehalose (8TMS); alpha-D-Glc-(1,1)-alpha-D-Glc
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:274002-11-1
RI:2748
RT:16.667
NUM PEAKS: 110
(71 5) (72 15) (73 1000) (74 83) (85 5)
(86 23) (87 11) (88 4) (89 6) (90 13)
(100 3) (101 7) (102 9) (103 22) (104 181)
(105 19) (106 7) (114 4) (115 17) (116 11)
(117 8) (118 16) (119 58) (120 6) (130 4)
(131 24) (132 151) (133 72) (134 16) (135 7)
(144 6) (145 8) (146 23) (147 268) (148 48)
(149 34) (150 4) (158 6) (159 5) (160 31)
(161 26) (162 5) (163 4) (164 4) (173 6)
(174 103) (175 15) (176 12) (177 10) (178 6)
(189 10) (190 4) (191 42) (192 254) (193 46)
(194 21) (204 3) (205 10) (206 92) (207 34)
(208 12) (209 3) (218 5) (219 8) (220 148)
(221 48) (222 20) (223 5) (232 4) (233 12)
(234 9) (235 14) (236 10) (237 4) (246 5)
(247 5) (248 52) (249 18) (250 9) (251 4)
(261 3) (262 6) (263 3) (264 5) (266 4)

(267 5) (276 4) (277 48) (278 10) (279 10)
(280 5) (293 5) (294 13) (295 5) (308 11)
(309 5) (310 3) (322 6) (323 17) (324 7)
(325 3) (336 15) (337 9) (338 4) (366 27)
(367 211) (368 69) (369 33) (370 7) (441 3)

NAME:13C_3269.3_1313EC16_Ergosterol (1TMS)
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:327001-11-1
RI:3269
RT:19.000
NUM PEAKS: 216
(70 52) (71 91) (72 223) (73 1000) (74 477)
(75 395) (76 47) (77 13) (80 16) (81 15)
(82 35) (83 92) (84 49) (85 151) (86 68)
(87 273) (88 97) (89 98) (90 9) (91 12)
(92 5) (93 7) (94 9) (95 8) (96 28)
(97 32) (98 180) (99 31) (100 117) (101 39)
(102 105) (103 45) (104 27) (105 5) (106 5)
(107 3) (109 6) (110 13) (111 24) (112 28)
(113 137) (114 23) (115 78) (116 34) (117 61)
(118 34) (119 12) (120 3) (122 6) (123 15)
(124 99) (125 30) (126 89) (127 43) (128 195)
(129 14) (130 32) (131 21) (132 94) (133 82)
(134 168) (135 18) (136 21) (137 59) (138 166)
(139 132) (140 42) (141 123) (142 22) (143 51)
(144 11) (145 22) (146 12) (147 23) (148 112)
(149 15) (150 20) (151 30) (152 159) (153 114)
(154 271) (155 58) (156 161) (157 20) (158 42)
(159 9) (160 26) (161 7) (162 10) (163 16)
(164 43) (165 59) (166 51) (167 133) (168 76)
(169 241) (170 70) (171 133) (172 12) (173 13)
(174 16) (175 37) (176 12) (177 17) (178 57)
(179 30) (180 55) (181 44) (182 111) (183 46)
(184 95) (185 17) (186 24) (187 6) (188 8)
(189 13) (190 7) (191 8) (192 21) (193 26)
(194 23) (195 57) (196 40) (197 102) (198 31)
(199 74) (200 11) (201 12) (202 9) (203 6)
(204 10) (205 5) (206 7) (207 7) (209 21)
(211 40) (212 102) (213 32) (214 63) (215 7)
(216 13) (217 3) (218 4) (219 5) (220 4)
(221 4) (222 4) (223 10) (224 14) (225 46)
(226 42) (227 138) (228 24) (229 46) (230 4)
(231 3) (232 8) (233 3) (237 3) (238 8)
(239 10) (240 26) (241 17) (242 34) (243 32)
(244 20) (245 4) (256 18) (257 30) (258 5)
(259 3) (268 7) (269 14) (270 49) (271 34)
(272 93) (273 5) (284 5) (285 14) (286 6)
(287 7) (298 3) (299 4) (300 9) (301 7)
(302 3) (304 3) (314 5) (315 8) (316 3)
(330 3) (332 3) (346 4) (347 3) (348 3)
(349 5) (358 5) (359 18) (360 40) (361 104)
(362 52) (363 8) (386 7) (387 24) (388 58)
(389 146) (390 68) (391 9) (403 8) (404 19)
(405 38) (406 18) (494 13) (495 27) (496 16)
(497 4)

NAME:13C_2109.4_1313EC11_
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:211004-11-1

RI:2109
RT:13.190
NUM PEAKS: 70
(72 29) (73 1000) (74 86) (75 98) (77 12)
(89 46) (90 11) (99 6) (102 16) (103 59)
(105 25) (115 14) (116 17) (117 15) (118 20)
(119 22) (130 9) (131 33) (132 122) (133 81)
(134 20) (135 19) (137 8) (146 11) (147 158)
(148 29) (149 21) (151 8) (157 4) (161 34)
(162 45) (163 16) (164 6) (165 4) (173 12)
(177 7) (181 10) (189 6) (191 12) (192 10)
(193 13) (195 10) (203 10) (205 11) (206 12)
(207 27) (211 57) (212 10) (219 12) (220 143)
(221 32) (222 11) (225 14) (227 16) (262 3)
(277 10) (298 11) (299 114) (300 36) (301 17)
(314 17) (315 176) (316 50) (317 25) (359 17)
(360 6) (367 5) (403 14) (404 7) (462 12)

NAME:13C_2114.1_1313EC11_
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:211003-11-1
RI:2114
RT:13.220
NUM PEAKS: 23
(70 8) (73 1000) (74 98) (75 120) (87 21)
(98 8) (103 55) (116 17) (131 26) (132 109)
(133 75) (146 11) (147 153) (173 10) (175 76)
(176 25) (220 103) (221 20) (285 6) (299 112)
(315 140) (316 37) (415 6)

NAME:13C_2125.1_1313EC11_
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:213003-11-1
RI:2125
RT:13.290
NUM PEAKS: 42
(72 22) (73 959) (74 81) (75 61) (87 150)
(89 19) (90 21) (101 69) (102 21) (103 35)
(104 78) (117 12) (119 54) (130 26) (131 30)
(132 38) (133 40) (134 14) (145 15) (147 176)
(148 30) (151 13) (160 16) (162 25) (175 1000)
(176 174) (177 74) (187 8) (189 17) (191 17)
(192 23) (206 36) (207 33) (220 41) (221 16)
(249 8) (298 14) (310 7) (369 10) (454 12)
(511 13) (532 12)

NAME:13C_2131.2_1313EC11_
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:213001-11-1
RI:2131
RT:13.328
NUM PEAKS: 160
(72 17) (73 1000) (74 76) (75 67) (85 14)
(86 6) (87 16) (88 6) (89 44) (90 24)
(92 3) (95 3) (96 3) (97 5) (100 5)
(101 13) (102 17) (103 21) (104 153) (105 23)
(106 6) (107 5) (110 4) (115 9) (116 27)
(117 7) (118 6) (119 73) (120 13) (128 4)
(131 28) (132 102) (133 55) (134 20) (135 7)
(137 4) (140 5) (145 9) (146 12) (147 250)

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(148   40) (149   27) (151    6) (154    3) (158    5)
(161   76) (162    9) (163   10) (164    4) (165    4)
(166    5) (167    3) (173    8) (174    4) (176    7)
(177    9) (178    8) (182    3) (186    4) (187    5)
(189    5) (191   30) (192   18) (198    3) (203    6)
(205    4) (206   36) (207  122) (208   19) (209   12)
(219    9) (220   91) (226    4) (228    3) (233   22)
(235    6) (239    3) (241    4) (250    3) (251    4)
(252    4) (253    3) (255    3) (259    6) (261    7)
(262    5) (264    8) (265   31) (266   10) (275    4)
(276    3) (279    5) (287    3) (288    6) (289    4)
(290    3) (293    4) (294   10) (302    4) (305    3)
(307    3) (308    5) (309    6) (310    8) (312    4)
(319    5) (320    6) (322   20) (323  145) (324   43)
(325   17) (329    4) (333    5) (334    5) (336    5)
(337    5) (338    7) (339    5) (342    3) (349    5)
(352    5) (358    3) (359    3) (361    3) (362    4)
(376    3) (377    5) (378    4) (379    5) (380    3)
(384    4) (389    3) (401    4) (409    3) (412    3)
(417    4) (425    3) (432    4) (433    5) (434    4)
(441    3) (448    6) (455    5) (456    5) (462    5)
(463    5) (465    3) (467    4) (468    4) (478    3)
(479    3) (500    5) (501    5) (505    4) (525    5)
(528    5) (534    3) (536    3) (540    3) (567    3)

NAME:13C_2155.1_1313EC11_
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:216003-11-1
RI:2155
RT:13.481
NUM PEAKS:  35
( 73 1000) ( 74   95) ( 86    9) ( 87   35) ( 90   22)
( 91   40) (104  176) (115   25) (118   20) (119   84)
(129   18) (131   31) (132   55) (133   50) (145   24)
(147  211) (148   36) (149   42) (157   10) (161   17)
(162   14) (174    8) (176   18) (177    7) (178   38)
(192    6) (203   21) (204   15) (207   55) (220   75)
(221   17) (235   25) (249    9) (352   25) (441    6)

NAME:13C_2162.2_1313EC11_
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:216002-11-1
RI:2162
RT:13.526
NUM PEAKS:  93
( 72   17) ( 73 1000) ( 74   83) ( 75   56) ( 86    6)
( 87  137) ( 88   11) ( 89   26) ( 90   15) (100    5)
(101   90) (102   14) (103   34) (104  157) (105   16)
(106    6) (115    7) (116    8) (117   13) (118    8)
(119   61) (120    5) (129    5) (130   15) (131   23)
(132   38) (133   40) (134   13) (135    4) (143    3)
(145   11) (146    9) (147  186) (148   31) (149   16)
(157    5) (159    8) (161   16) (173   30) (174   12)
(175  250) (176   43) (177   20) (178    3) (187   13)
(188    5) (189    5) (191   22) (192    8) (201    4)
(202    6) (203    6) (204    4) (205    3) (206   16)
(207   45) (208    8) (217    8) (218    4) (219   12)
(220   96) (221   20) (222    8) (233    5) (245   19)
(260    4) (261    6) (273    7) (274   18) (275    5)
(276    3) (279    6) (290   16) (291    6) (294    3)
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(304 5) (305 4) (306 4) (307 3) (308 8)
(309 4) (310 17) (311 5) (318 10) (319 12)
(320 5) (323 6) (335 6) (349 11) (350 3)
(435 3) (525 5) (526 4)

NAME:13C_2168.8_1313EC11_
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:217002-11-1
RI:2169
RT:13.568
NUM PEAKS: 18
(73 1000) (74 83) (75 81) (87 57) (101 31)
(103 14) (132 37) (133 38) (145 24) (147 173)
(148 28) (149 16) (174 10) (191 14) (192 34)
(220 34) (262 41) (442 38)

NAME:13C_2179.9_1313EC11_
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:218001-11-1
RI:2180
RT:13.638
NUM PEAKS: 57
(72 24) (73 1000) (74 88) (75 135) (87 30)
(88 12) (89 32) (90 20) (100 15) (103 27)
(104 190) (105 22) (115 8) (116 13) (117 13)
(118 28) (119 72) (130 8) (131 27) (132 50)
(133 55) (134 19) (145 27) (146 21) (147 222)
(148 40) (149 57) (150 7) (161 13) (162 24)
(163 12) (176 23) (177 10) (178 52) (179 5)
(188 9) (189 8) (203 26) (205 7) (207 42)
(220 78) (221 22) (222 9) (234 7) (235 18)
(236 6) (249 9) (275 4) (319 5) (320 6)
(322 8) (348 7) (351 10) (352 34) (353 9)
(528 8) (533 3)

NAME:13C_2217.6_1313EC11_9-(Z)-Octadecenoic acid (1TMS)
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:222001-11-1
RI:2218
RT:13.859
NUM PEAKS: 98
(70 29) (71 32) (72 257) (73 606) (74 268)
(75 1000) (76 84) (77 49) (83 25) (84 20)
(85 102) (86 54) (87 189) (88 122) (89 251)
(90 17) (91 14) (93 4) (96 3) (97 4)
(98 35) (99 10) (100 63) (101 56) (102 244)
(103 131) (104 157) (105 8) (106 11) (113 14)
(114 9) (115 36) (116 52) (117 93) (118 163)
(119 573) (120 44) (121 15) (128 24) (130 35)
(131 52) (132 541) (133 57) (134 203) (135 32)
(136 8) (143 18) (144 19) (145 27) (146 44)
(148 190) (149 19) (150 6) (158 13) (159 13)
(160 26) (161 31) (162 47) (163 25) (164 3)
(173 6) (174 3) (176 19) (177 29) (178 26)
(179 5) (180 3) (188 5) (190 19) (191 26)
(192 30) (193 35) (194 8) (205 5) (206 62)
(208 11) (221 6) (222 9) (223 5) (236 22)
(237 13) (238 30) (250 3) (251 7) (252 10)
(253 5) (266 4) (268 5) (281 5) (282 28)
(283 5) (284 3) (355 9) (356 23) (357 91)

(358 12) (359 5) (372 6)

NAME:13C_2224.7_1313EC11_Octadecenoic acid (1TMS)
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:223003-11-1
RI:2225
RT:13.897
NUM PEAKS: 101
(70 36) (71 36) (72 267) (73 936) (74 286)
(75 1000) (76 88) (83 30) (84 24) (85 95)
(86 57) (87 209) (88 111) (89 245) (90 21)
(96 6) (98 39) (99 13) (100 66) (101 108)
(102 270) (103 134) (104 134) (106 15) (113 18)
(114 10) (115 38) (116 55) (117 111) (118 169)
(119 530) (120 36) (121 18) (128 28) (129 14)
(130 39) (131 67) (132 520) (133 62) (143 22)
(144 22) (145 25) (146 44) (147 31) (148 191)
(149 30) (156 11) (159 17) (160 24) (161 34)
(162 50) (163 25) (169 6) (173 10) (175 16)
(176 24) (177 40) (178 24) (180 5) (187 6)
(188 11) (189 11) (190 16) (191 28) (192 29)
(193 29) (203 31) (204 18) (205 14) (208 12)
(217 9) (219 24) (235 7) (236 21) (237 12)
(238 27) (247 4) (248 4) (251 5) (267 8)
(269 9) (281 5) (282 26) (292 6) (293 47)
(294 18) (295 9) (309 3) (327 5) (328 4)
(347 5) (356 18) (357 90) (358 11) (360 5)
(372 8) (384 8) (416 9) (425 3) (434 5)
(523 5)

NAME:13C_2343.5_1313EC11_
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:234001-11-1
RI:2344
RT:14.526
NUM PEAKS: 23
(72 22) (73 1000) (74 82) (75 101) (100 25)
(104 58) (119 22) (131 26) (132 34) (133 50)
(144 18) (147 145) (148 29) (218 21) (219 14)
(220 370) (221 64) (222 29) (270 25) (357 18)
(358 45) (373 10) (386 6)

NAME:13C_2383.1_1313EC11_
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:238002-11-1
RI:2383
RT:14.735
NUM PEAKS: 24
(72 36) (73 1000) (74 89) (75 107) (89 24)
(90 25) (103 29) (104 158) (118 13) (119 175)
(131 27) (132 43) (133 36) (147 211) (148 35)
(149 19) (161 22) (162 65) (163 22) (173 18)
(191 19) (206 13) (207 37) (220 73)

NAME:13C_2475.1_1313EC11_
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:248002-11-1
RI:2475
RT:15.223
NUM PEAKS: 120

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( 70   16) ( 72   29) ( 73 1000) ( 74   86) ( 75  131)
( 77   10) ( 82    5) ( 83    7) ( 84    4) ( 86    9)
( 87   12) ( 88    5) ( 89    8) ( 90   14) ( 95    5)
( 96    5) ( 97    5) ( 98    5) ( 99   40) (100   15)
(101   13) (102   18) (103   31) (104  125) (105   15)
(106    5) (112    6) (113    8) (114   10) (115   10)
(116   12) (117   29) (118   12) (119   27) (120    3)
(125    3) (126   10) (127    4) (128    3) (129    4)
(130    4) (131   26) (132   72) (133   72) (135    8)
(139    4) (140    7) (141    3) (144    6) (145    8)
(146   24) (147  156) (148   30) (149   30) (153   17)
(154    3) (155    7) (156    6) (158    9) (159    4)
(160    6) (161   11) (164    4) (168    3) (169   61)
(170   18) (171    6) (173    5) (174   58) (175    9)
(176   12) (177    3) (178    3) (183    7) (184    4)
(185   26) (186    4) (191   15) (192   21) (193    5)
(196   14) (199    3) (206   13) (213   12) (214   20)
(215    4) (218   12) (219   16) (220  303) (221   65)
(222   30) (223    4) (227    3) (228    5) (229    3)
(233    5) (234   16) (235   13) (236    4) (241    4)
(242    4) (243    3) (245   12) (248   22) (249   15)
(250    5) (255    3) (257    5) (263    6) (264   62)
(265   11) (266    5) (270   11) (271    7) (272    3)
(301   12) (302    3) (317    7) (353    3) (450    3)

NAME:13C_2732.8_1313EC11_
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:273002-11-1
RI:2733
RT:16.587
NUM PEAKS:  64
( 71    6) ( 72   16) ( 73 1000) ( 74   89) ( 75   85)
( 84    5) ( 86   25) ( 87   11) ( 89   31) ( 90   16)
(101   11) (102    8) (103   27) (104  123) (105   36)
(106    8) (115   10) (116    9) (117    9) (118   13)
(119   76) (121    5) (131   21) (132   90) (133   56)
(134   21) (145    6) (146   23) (147  259) (148   46)
(149   27) (160   15) (161   16) (162   83) (163   20)
(173    8) (174   52) (175    8) (178    8) (189    5)
(190   10) (191   25) (192   34) (193    9) (205    9)
(206  244) (207  107) (208   26) (220  122) (221   32)
(222   11) (234    7) (248   44) (249   12) (275    3)
(277   23) (278    9) (294    6) (323   18) (366   22)
(367  132) (368   40) (369   18) (396    4)

NAME:13C_2814.8_1313EC11_
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:281001-11-1
RI:2815
RT:17.009
NUM PEAKS:  53
( 72   14) ( 73 1000) ( 74   83) ( 75   81) ( 87    9)
( 89   25) (103   40) (104   74) (105   20) (106    6)
(115   10) (118   18) (119   52) (131   22) (132   81)
(133   56) (134   20) (135    7) (145   10) (146   18)
(147  273) (148   47) (149   30) (161   17) (162   67)
(164   30) (174   37) (176    6) (191   32) (192   42)
(206  264) (207  106) (208   28) (219    9) (220   80)
(221  176) (222   45) (223   20) (236    6) (248   19)
(249   11) (264    7) (279    6) (281   30) (282    9)
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(295 48) (296 16) (323 9) (324 5) (355 8)
(367 85) (368 29) (369 34)

NAME:13C_2825.9_1313EC11_
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:283001-11-1
RI:2826
RT:17.058
NUM PEAKS: 36
(70 27) (72 174) (73 189) (74 1000) (83 45)
(86 53) (87 511) (88 20) (89 18) (98 59)
(100 109) (101 43) (102 144) (104 8) (113 35)
(114 12) (115 71) (117 59) (128 31) (129 16)
(130 92) (131 19) (132 58) (143 20) (144 20)
(145 49) (146 75) (147 59) (158 26) (160 44)
(171 7) (173 15) (175 8) (203 11) (205 10)
(218 10)

NAME:13C_2872.6_1313EC11_Isomaltose methoxyamine (8TMS); alpha-D-Glc-(1,6)-D-Glc (8TMS)
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:287001-11-1
RI:2873
RT:17.266
NUM PEAKS: 58
(73 1000) (74 87) (75 98) (76 9) (86 17)
(87 12) (88 5) (89 30) (90 12) (101 21)
(102 13) (103 42) (104 112) (105 28) (115 14)
(116 13) (118 21) (119 67) (130 7) (131 21)
(132 115) (133 65) (134 23) (135 9) (145 11)
(146 21) (147 236) (148 41) (149 27) (160 19)
(161 26) (162 89) (163 17) (164 25) (173 8)
(174 61) (175 10) (177 9) (190 6) (191 35)
(192 49) (205 13) (206 207) (207 59) (208 22)
(220 115) (234 13) (235 17) (248 29) (249 14)
(277 23) (278 9) (279 8) (323 16) (366 24)
(367 140) (368 46) (369 21)

NAME:13C_2907.8_1313EC11_Isomaltose methoxyamine (BP) (8TMS); alpha-D-Glc-(1,6)-D-Glc (8TMS)
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:291002-11-1
RI:2908
RT:17.423
NUM PEAKS: 72
(72 14) (73 1000) (74 83) (75 111) (79 18)
(86 23) (87 14) (89 24) (90 13) (94 12)
(98 13) (102 23) (103 44) (104 140) (105 26)
(115 18) (117 12) (118 12) (119 48) (126 10)
(131 21) (132 93) (133 55) (134 37) (146 26)
(147 221) (148 40) (160 13) (161 23) (162 74)
(164 33) (165 15) (174 61) (178 9) (191 26)
(192 41) (204 12) (206 200) (207 63) (212 9)
(220 87) (221 19) (233 9) (235 34) (248 31)
(251 10) (259 8) (262 10) (270 8) (279 14)
(289 11) (308 20) (309 12) (310 15) (314 9)
(322 10) (340 12) (366 21) (367 128) (368 43)
(381 18) (389 14) (397 8) (411 12) (412 7)
(420 9) (437 17) (448 15) (534 9) (536 10)
(545 9) (577 6)

NAME:13C_2932.1_1313EC11_
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:293001-11-1
RI:2932
RT:17.530
NUM PEAKS: 96
(72 14) (73 1000) (74 83) (75 83) (76 4)
(81 8) (86 10) (87 8) (88 4) (89 5)
(90 6) (101 7) (102 7) (103 79) (104 81)
(105 10) (111 3) (115 8) (116 6) (117 9)
(118 15) (119 36) (129 62) (130 8) (131 22)
(132 78) (133 64) (134 10) (135 5) (143 11)
(144 4) (145 7) (146 15) (147 299) (148 47)
(149 32) (150 3) (157 7) (160 8) (161 14)
(174 28) (175 7) (176 4) (177 6) (178 3)
(189 9) (190 6) (191 166) (192 66) (193 19)
(194 3) (204 15) (205 22) (206 591) (207 108)
(208 46) (209 5) (217 49) (218 11) (219 9)
(220 90) (221 38) (222 12) (230 16) (231 6)
(232 3) (233 3) (234 4) (235 7) (243 6)
(247 4) (248 15) (249 5) (265 4) (271 3)
(277 7) (278 3) (291 5) (293 7) (294 5)
(304 4) (305 16) (306 6) (307 3) (308 8)
(309 3) (318 9) (319 6) (322 4) (323 4)
(336 3) (343 5) (367 20) (368 6) (433 10)
(434 5)

NAME:13C_2517.7_1313EC11_
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:252002-11-1
RI:2518
RT:15.448
NUM PEAKS: 254
(70 14) (71 36) (72 107) (73 1000) (74 97)
(75 126) (76 10) (77 7) (78 3) (79 3)
(83 10) (84 7) (85 32) (86 12) (87 15)
(88 11) (89 32) (90 19) (91 6) (93 4)
(96 3) (97 6) (98 7) (99 9) (100 11)
(101 53) (102 26) (103 33) (104 185) (105 20)
(106 6) (108 3) (111 6) (112 4) (113 13)
(114 9) (115 10) (116 11) (117 9) (118 11)
(119 57) (120 6) (121 3) (124 3) (125 3)
(127 4) (129 14) (130 9) (131 27) (132 45)
(133 51) (134 18) (135 9) (137 3) (138 3)
(140 4) (141 7) (142 7) (143 6) (144 9)
(145 22) (146 20) (147 191) (148 32) (149 20)
(150 4) (151 4) (153 3) (154 3) (155 4)
(157 4) (158 8) (159 9) (160 90) (161 21)
(162 12) (163 8) (164 3) (169 3) (171 5)
(172 9) (173 11) (174 8) (175 25) (176 38)
(177 16) (178 5) (180 4) (183 3) (186 6)
(187 7) (188 7) (189 6) (190 6) (191 72)
(192 17) (193 7) (195 3) (196 5) (197 3)
(198 3) (201 4) (202 4) (203 7) (204 8)
(205 5) (206 15) (207 28) (208 7) (209 5)
(212 4) (213 5) (214 4) (215 3) (216 6)
(217 3) (218 6) (219 14) (220 114) (221 20)
(222 9) (223 3) (226 3) (227 4) (230 3)
(231 7) (232 16) (233 8) (234 6) (235 6)

(236 4) (239 3) (244 3) (245 7) (246 4)
(247 4) (248 9) (249 6) (250 4) (253 5)
(257 3) (260 3) (261 4) (262 5) (263 3)
(264 5) (265 3) (266 3) (267 3) (268 3)
(274 3) (276 4) (277 7) (278 4) (279 12)
(280 4) (289 3) (293 4) (294 6) (295 3)
(296 3) (301 4) (302 3) (304 3) (305 4)
(306 7) (307 4) (308 4) (309 3) (310 5)
(313 3) (319 3) (320 8) (321 3) (322 5)
(323 5) (324 5) (325 3) (326 3) (333 3)
(334 4) (335 6) (336 5) (337 3) (338 3)
(339 3) (341 3) (344 3) (347 3) (349 5)
(350 7) (351 21) (352 9) (353 3) (361 3)
(363 3) (364 5) (365 4) (367 3) (368 3)
(372 3) (376 3) (377 3) (380 4) (381 12)
(382 11) (383 3) (387 4) (388 3) (394 3)
(395 4) (396 4) (397 3) (409 3) (412 3)
(422 6) (423 16) (424 10) (425 5) (427 3)
(437 3) (439 3) (442 3) (447 3) (449 3)
(450 3) (452 6) (453 20) (454 56) (455 26)
(456 10) (457 3) (460 3) (467 3) (470 3)
(480 3) (481 3) (491 3) (492 3) (503 3)
(506 3) (508 3) (513 4) (514 4) (515 3)
(516 4) (519 3) (522 3) (526 4) (535 3)
(536 3) (542 3) (544 3) (569 3)

NAME:13C_2491.6_1313EC11_
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:249001-11-1
RI:2492
RT:15.310
NUM PEAKS: 205
(70 15) (71 16) (72 60) (73 1000) (74 66)
(75 104) (77 10) (82 4) (85 15) (86 7)
(87 5) (88 3) (89 14) (90 10) (92 5)
(93 3) (96 7) (98 3) (99 10) (100 11)
(101 27) (102 12) (103 28) (104 121) (105 16)
(106 7) (108 5) (110 3) (111 4) (113 3)
(114 7) (115 4) (116 6) (117 7) (118 5)
(119 27) (123 4) (126 6) (128 3) (129 7)
(131 27) (132 16) (133 42) (134 7) (139 6)
(141 4) (142 6) (143 6) (144 4) (145 22)
(146 13) (147 208) (148 41) (149 22) (150 3)
(151 3) (155 4) (158 4) (159 3) (160 52)
(161 16) (162 7) (163 6) (168 4) (169 10)
(170 4) (171 4) (172 5) (173 5) (174 16)
(175 11) (176 25) (177 5) (185 8) (186 3)
(188 7) (189 4) (191 32) (192 12) (193 5)
(194 4) (195 3) (196 3) (202 4) (203 6)
(204 3) (205 8) (206 4) (207 33) (208 8)
(210 4) (211 3) (213 3) (214 6) (216 5)
(218 3) (219 6) (220 98) (221 52) (222 14)
(223 7) (231 4) (232 11) (233 5) (234 7)
(235 5) (236 3) (237 3) (239 3) (245 3)
(248 4) (249 5) (252 6) (256 4) (257 4)
(258 4) (261 5) (263 3) (264 12) (265 5)
(266 4) (267 7) (270 4) (273 4) (274 3)
(275 4) (276 7) (277 3) (279 10) (280 3)
(281 20) (282 3) (283 3) (288 5) (295 6)
(309 3) (310 4) (317 5) (319 8) (320 9)

(321 3)	(323 5)	(325 8)	(326 3)	(329 3)
(334 3)	(335 3)	(341 7)	(342 4)	(347 3)
(348 4)	(350 5)	(351 19)	(352 7)	(353 3)
(355 18)	(356 9)	(357 4)	(364 3)	(374 4)
(378 4)	(381 12)	(382 6)	(383 3)	(389 3)
(390 3)	(394 4)	(398 3)	(400 3)	(401 4)
(418 3)	(419 3)	(422 5)	(423 12)	(424 6)
(425 4)	(429 5)	(430 6)	(431 5)	(434 3)
(435 5)	(438 3)	(439 4)	(449 5)	(450 4)
(452 7)	(453 19)	(454 53)	(455 20)	(456 8)
(459 4)	(471 4)	(474 5)	(481 6)	(490 4)
(491 5)	(505 4)	(528 3)	(534 3)	(541 3)
(543 3)	(557 3)	(562 4)	(569 3)	(592 3)

NAME:13C_3307.7_1313EC07_
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:331001-11-1
RI:3308
RT:19.156
NUM PEAKS: 141

(72 135)	(73 765)	(74 279)	(75 626)	(76 387)
(77 49)	(82 9)	(83 13)	(85 29)	(86 28)
(87 205)	(88 75)	(89 209)	(90 49)	(91 189)
(93 17)	(98 19)	(100 45)	(101 29)	(102 198)
(103 128)	(104 381)	(105 53)	(106 38)	(113 12)
(115 38)	(116 38)	(117 55)	(118 102)	(119 144)
(120 23)	(121 16)	(122 7)	(128 15)	(129 12)
(130 21)	(131 34)	(132 1000)	(133 149)	(134 283)
(135 40)	(136 24)	(141 12)	(142 9)	(145 24)
(147 90)	(148 847)	(149 109)	(150 39)	(156 9)
(157 7)	(158 9)	(160 11)	(161 23)	(162 17)
(163 26)	(164 47)	(165 298)	(171 11)	(175 15)
(177 19)	(178 15)	(179 26)	(183 6)	(189 7)
(192 19)	(193 37)	(194 80)	(195 10)	(207 82)
(208 13)	(209 9)	(211 6)	(220 7)	(221 8)
(222 18)	(224 9)	(229 8)	(230 10)	(232 8)
(234 8)	(237 33)	(238 43)	(239 460)	(240 36)
(241 19)	(242 23)	(244 9)	(248 10)	(250 8)
(252 25)	(253 30)	(254 30)	(255 118)	(256 8)
(267 35)	(282 10)	(285 14)	(289 11)	(291 8)
(299 8)	(308 10)	(309 7)	(311 9)	(312 15)
(313 26)	(314 57)	(315 9)	(325 7)	(328 25)
(329 113)	(330 17)	(331 8)	(332 13)	(334 8)
(343 10)	(344 24)	(345 27)	(357 11)	(358 11)
(375 7)	(381 9)	(391 9)	(392 9)	(402 9)
(403 35)	(404 33)	(408 6)	(428 11)	(461 12)
(493 5)	(497 7)	(498 7)	(501 6)	(508 7)
(511 8)	(523 6)	(569 11)	(570 24)	(571 11)
(573 4)				

NAME:13C_3401.6_1313EC07_
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:340002-11-1
RI:3402
RT:19.533
NUM PEAKS: 214

(70 188)	(71 791)	(72 275)	(73 872)	(74 1000)
(75 556)	(76 73)	(77 48)	(80 27)	(81 45)
(82 68)	(83 290)	(84 120)	(85 663)	(86 70)
(87 255)	(88 54)	(89 120)	(91 28)	(95 20)

```
( 96   56) ( 97  193) ( 98  289) ( 99  243) (100  230)
(101   48) (102  278) (103   49) (104   32) (106    7)
(109    9) (110   34) (111  108) (112   70) (113  399)
(114   43) (115  196) (116   27) (117  179) (118   11)
(119   48) (120   16) (123   13) (124   73) (125   75)
(126  120) (127  124) (128  191) (129   35) (130  133)
(131   55) (132  358) (133   43) (134   36) (137   35)
(138   70) (139  100) (140   67) (141  228) (142   55)
(143  167) (144   87) (145  429) (146   76) (148   18)
(149   12) (152   54) (153   46) (154  103) (155   92)
(156  151) (157   85) (158  143) (159   43) (160  100)
(162   31) (164   23) (165   17) (166   21) (167   42)
(168   48) (169  114) (170   36) (171  129) (172   38)
(173  114) (174   29) (175   57) (176    9) (177   23)
(178   15) (179   13) (180   16) (181   17) (182   30)
(183   38) (184   57) (185   34) (186   99) (187   38)
(188   94) (189   21) (190   37) (191    9) (192   14)
(196   20) (197   53) (198   12) (199   58) (200   49)
(201  107) (202   30) (203   47) (207   17) (208   10)
(210   10) (211   28) (212   24) (213   16) (214   42)
(215   12) (216   56) (217   19) (218   41) (219   26)
(220   46) (221   11) (224   12) (225   19) (226   12)
(227   15) (228   11) (229   33) (230   16) (231   26)
(232   11) (234   13) (235   34) (238    9) (239   17)
(240   13) (241    8) (243    8) (245   10) (246   20)
(251   12) (253   14) (256   14) (259   63) (260   10)
(261   46) (262   18) (263   19) (266   14) (272    8)
(273   10) (274   24) (275   18) (276   29) (277   51)
(278   22) (282   10) (286   10) (288   11) (289   11)
(290    9) (291   12) (292   16) (302   14) (309   10)
(319   14) (320    9) (322   10) (323    8) (324    8)
(327   10) (332   11) (334   10) (335   13) (338   14)
(342   12) (349   16) (361    7) (377   11) (379   12)
(380   15) (391    9) (392   12) (394   10) (405   11)
(406   13) (407   43) (422   13) (423   25) (424   12)
(429   15) (442    6) (451   11) (452    9) (455    7)
(468   13) (476   11) (495    7) (499    9) (512   24)
(513   45) (514   13) (518    8) (523    6) (545   10)
(546    9) (547    8) (566    8) (592    6)

NAME:13C_3494.1_1313EC07_
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:349001-11-1
RI:3494
RT:19.905
NUM PEAKS:  70
( 70   20) ( 72  144) ( 73  864) ( 74  282) ( 75  770)
( 76  360) ( 77   71) ( 86   28) ( 87  149) ( 88   94)
( 89  300) ( 90   62) ( 91  155) ( 92   14) ( 93   25)
(100   23) (101   40) (102  230) (103  134) (104  457)
(105   36) (106   47) (116   37) (117  129) (118  107)
(119  148) (120   30) (122   20) (130   19) (131   25)
(132 1000) (133  166) (134  281) (135   29) (136   22)
(146   21) (147   65) (148  858) (149  130) (150   20)
(162   23) (168   12) (177   35) (179   15) (192   26)
(193   51) (194  114) (195  217) (207   78) (222   17)
(252   15) (255   43) (267   38) (268   49) (269  376)
(270   30) (271   16) (284   13) (285   45) (328   26)
(329  140) (343   21) (344   73) (345   40) (403   32)
(404   43) (424   12) (425   12) (473   10) (572    9)
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NAME:13C_3334.7_1313EC07_
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:334001-11-1
RI:3335
RT:19.264
NUM PEAKS: 191
(70 67) (71 41) (72 226) (73 1000) (74 566)
(75 796) (76 188) (77 53) (80 29) (82 43)
(83 123) (84 46) (85 184) (86 56) (87 294)
(88 66) (89 119) (91 57) (92 23) (93 24)
(94 21) (95 33) (96 37) (97 46) (98 274)
(99 40) (100 189) (101 54) (102 240) (103 57)
(104 89) (105 16) (111 39) (113 267) (114 31)
(115 147) (116 53) (117 137) (118 34) (119 51)
(123 25) (124 120) (125 33) (126 138) (127 75)
(128 328) (129 63) (130 137) (131 43) (132 156)
(133 59) (134 156) (135 21) (136 20) (137 82)
(138 184) (139 182) (140 57) (141 209) (142 70)
(143 142) (144 47) (145 84) (146 45) (148 118)
(150 22) (151 40) (152 155) (153 144) (154 364)
(155 109) (156 333) (157 62) (158 100) (159 24)
(160 57) (161 21) (162 20) (164 56) (166 63)
(167 148) (168 80) (169 268) (170 141) (171 212)
(172 49) (173 77) (174 33) (175 60) (176 16)
(177 19) (178 51) (179 28) (180 46) (181 49)
(182 126) (183 58) (184 158) (185 58) (186 88)
(187 31) (188 32) (189 29) (190 16) (192 24)
(193 38) (194 19) (195 55) (196 37) (197 106)
(198 48) (199 126) (201 45) (203 29) (204 23)
(210 50) (211 46) (212 105) (213 60) (214 108)
(215 23) (217 17) (219 42) (220 19) (222 27)
(225 23) (226 31) (227 128) (228 43) (229 54)
(230 29) (232 15) (240 23) (241 24) (242 53)
(243 50) (244 65) (246 24) (251 17) (252 15)
(253 12) (256 15) (257 16) (258 15) (259 35)
(260 18) (261 30) (271 24) (272 58) (273 15)
(284 17) (285 26) (287 19) (289 11) (292 13)
(300 17) (302 18) (309 22) (334 15) (342 9)
(350 16) (352 14) (362 38) (363 83) (364 112)
(365 15) (368 14) (377 20) (379 16) (380 14)
(386 20) (390 28) (391 108) (392 163) (393 42)
(395 13) (405 22) (406 16) (407 33) (408 33)
(435 14) (444 17) (483 21) (484 15) (494 14)
(497 32) (498 35) (499 13) (509 17) (533 13)
(568 8)

NAME:13C_3347.5_1313EC07_
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:335001-11-1
RI:3348
RT:19.315
NUM PEAKS: 140
(70 55) (71 36) (72 231) (73 535) (74 433)
(75 1000) (76 66) (77 32) (82 27) (83 125)
(84 52) (85 242) (86 45) (87 264) (88 32)
(89 123) (90 83) (96 18) (97 27) (98 317)
(99 50) (100 206) (101 59) (102 190) (103 26)
(104 35) (111 31) (112 34) (113 297) (114 55)
(115 243) (116 33) (117 83) (123 12) (124 73)

(125 24) (126 123) (127 39) (128 179) (129 44)
(130 85) (131 30) (132 64) (133 12) (136 10)
(137 29) (138 73) (139 100) (140 37) (141 180)
(142 51) (143 131) (144 45) (145 64) (146 17)
(152 53) (153 47) (154 108) (155 50) (156 173)
(157 58) (158 117) (159 19) (160 54) (161 55)
(162 18) (166 21) (167 39) (168 21) (169 88)
(170 42) (171 145) (172 29) (173 70) (174 24)
(175 25) (178 8) (180 11) (181 18) (182 35)
(184 66) (185 18) (186 70) (187 23) (188 24)
(189 17) (190 26) (191 8) (195 8) (197 26)
(198 15) (199 63) (200 27) (201 39) (202 13)
(203 31) (204 24) (212 34) (213 19) (214 43)
(216 36) (217 27) (218 15) (226 13) (227 51)
(228 27) (229 112) (230 14) (231 15) (242 21)
(243 28) (244 78) (245 27) (257 16) (258 14)
(259 11) (261 12) (270 6) (271 21) (272 86)
(276 7) (278 7) (302 25) (303 9) (317 16)
(347 20) (348 11) (361 46) (362 210) (363 44)
(364 14) (391 15) (392 29) (393 18) (407 20)
(408 51) (409 13) (482 17) (483 9) (530 8)

NAME:13C_3353.6_1313EC07_
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:335002-11-1
RI:3354
RT:19.340
NUM PEAKS: 166
(70 62) (71 62) (72 175) (73 888) (74 215)
(75 1000) (76 232) (77 67) (83 148) (84 65)
(85 190) (86 23) (87 321) (88 34) (89 79)
(90 28) (91 37) (93 37) (97 41) (98 344)
(99 52) (100 177) (101 42) (102 209) (104 129)
(105 34) (106 29) (110 30) (111 47) (112 31)
(113 284) (114 43) (115 169) (117 104) (118 51)
(119 23) (121 17) (124 53) (125 26) (126 88)
(127 44) (128 159) (129 72) (130 92) (132 103)
(134 48) (137 43) (138 67) (139 82) (140 48)
(141 161) (142 41) (143 126) (144 100) (145 109)
(146 36) (147 181) (150 32) (152 76) (153 64)
(154 120) (155 63) (156 141) (157 49) (158 145)
(160 60) (161 17) (162 25) (163 24) (165 30)
(166 46) (169 102) (170 57) (171 120) (172 25)
(173 79) (174 23) (179 28) (184 37) (185 26)
(186 84) (188 57) (190 19) (192 34) (197 24)
(198 25) (199 44) (200 51) (206 50) (207 74)
(212 40) (213 28) (214 51) (215 56) (216 27)
(217 16) (218 27) (220 61) (221 117) (222 31)
(223 42) (227 33) (228 58) (229 198) (230 26)
(231 33) (233 20) (245 41) (246 104) (253 37)
(259 22) (274 226) (276 31) (280 18) (281 49)
(293 30) (300 25) (308 19) (316 26) (320 39)
(333 23) (342 18) (357 30) (375 22) (377 28)
(379 24) (381 32) (382 19) (394 46) (400 26)
(417 33) (420 34) (421 20) (425 16) (426 31)
(429 25) (430 23) (433 13) (440 25) (441 37)
(445 27) (449 16) (450 23) (455 30) (457 24)
(484 38) (487 22) (499 51) (500 109) (501 42)
(502 17) (515 29) (516 39) (520 16) (524 29)
(525 21) (529 18) (534 18) (537 18) (545 17)

(568 12) (569 10) (574 11) (587 11) (590 14)
(599 7)

NAME:13C_2654.6_1313EC07_
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:266001-11-1
RI:2655
RT:16.184
NUM PEAKS: 100
(70 7) (71 12) (72 70) (73 1000) (74 328)
(75 86) (85 29) (86 16) (87 60) (88 13)
(89 33) (90 12) (99 8) (100 14) (101 27)
(102 32) (103 86) (104 312) (105 15) (106 8)
(114 8) (115 28) (116 13) (118 24) (119 67)
(120 6) (128 10) (129 7) (130 10) (131 69)
(132 55) (133 204) (134 8) (143 8) (144 14)
(145 13) (146 14) (147 210) (148 31) (149 15)
(157 11) (158 7) (159 20) (160 17) (172 11)
(173 33) (174 27) (175 30) (176 49) (177 15)
(187 18) (189 13) (190 28) (191 19) (192 9)
(202 5) (203 16) (204 23) (205 10) (206 32)
(207 24) (208 4) (213 11) (216 6) (218 9)
(219 9) (220 37) (221 8) (224 4) (231 9)
(232 12) (233 10) (245 5) (246 9) (247 12)
(273 6) (274 41) (275 22) (276 37) (277 15)
(294 4) (295 7) (301 4) (302 12) (303 60)
(304 15) (306 12) (307 61) (308 7) (320 10)
(334 22) (335 18) (336 42) (337 12) (338 7)
(393 15) (410 4) (482 6) (483 17) (484 7)

NAME:13C_2689.6_1313EC07_
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:269002-11-1
RI:2690
RT:16.369
NUM PEAKS: 259
(70 5) (71 13) (72 10) (73 1000) (74 86)
(75 48) (76 13) (77 3) (78 3) (82 4)
(83 3) (84 21) (85 20) (86 47) (87 12)
(88 13) (90 19) (93 18) (96 7) (97 28)
(99 20) (100 13) (101 7) (103 42) (104 287)
(105 56) (108 19) (115 12) (116 4) (117 37)
(118 18) (119 23) (120 7) (121 4) (127 17)
(128 4) (130 6) (132 216) (133 51) (134 6)
(139 7) (140 4) (143 19) (145 9) (146 26)
(147 259) (148 70) (149 12) (150 20) (151 4)
(154 7) (156 22) (157 11) (160 66) (161 43)
(164 8) (168 8) (169 3) (170 9) (171 14)
(174 187) (175 32) (176 29) (177 34) (178 5)
(179 8) (182 4) (184 11) (187 9) (188 7)
(189 6) (190 8) (191 81) (192 427) (193 69)
(194 17) (199 16) (200 26) (201 11) (204 7)
(205 38) (206 335) (209 4) (215 8) (216 16)
(217 12) (220 231) (221 32) (222 10) (231 11)
(232 9) (233 7) (235 36) (236 13) (238 4)
(244 19) (246 4) (247 15) (248 66) (249 7)
(250 5) (251 8) (252 9) (254 6) (255 13)
(256 7) (257 19) (258 8) (259 4) (260 3)
(262 12) (263 6) (264 22) (265 7) (266 3)
(272 5) (274 5) (278 6) (282 21) (285 4)

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(291   20) (292    3) (293   16) (294   15) (305   13)
(306   13) (307   21) (308   16) (309    4) (310   11)
(312    3) (320   13) (321    4) (322   16) (323   21)
(326    4) (327   17) (331    6) (332   12) (334    4)
(336   11) (338    3) (339    6) (340    8) (341    9)
(342    6) (343    3) (345    5) (346    5) (347    4)
(352    8) (361    5) (363   10) (365    3) (366   63)
(367  353) (368  103) (369   50) (370   19) (375    4)
(378    7) (379   15) (382   15) (391   10) (397   11)
(398   14) (399    5) (400    6) (403   21) (404    7)
(405    5) (406    8) (407   16) (409   12) (417    3)
(418    3) (419    6) (423    3) (424    7) (425    7)
(427   15) (428   11) (429   10) (430    4) (433   25)
(434   14) (437   11) (438    5) (439    5) (441    4)
(442    8) (450    3) (451    4) (454    7) (456   14)
(457   11) (458    6) (460   11) (461   14) (462    8)
(464    5) (466   11) (469   11) (473   15) (474   22)
(477    3) (480    3) (481   11) (482    5) (486    7)
(487    6) (489   14) (491    6) (494    6) (496    5)
(502    4) (505    6) (506    7) (508   12) (511   15)
(512   10) (514    7) (515   15) (516   11) (518    8)
(519   11) (522    3) (524   16) (526   12) (528   14)
(529   28) (533    4) (535    6) (538    8) (539    6)
(550    5) (552    7) (553    6) (556   11) (560    4)
(561   14) (563    8) (564    3) (565    6) (567   11)
(574    7) (575    8) (576    6) (581    7) (588    8)
(591    4) (593    3) (594    4) (597    8)
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NAME:13C_2617.8_1313EC07_
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:262001-11-1
RI:2618
RT:15.988
NUM PEAKS:  116
( 70    5) ( 71    6) ( 72   19) ( 73 1000) ( 74   89)
( 75  141) ( 76    9) ( 77   10) ( 85    5) ( 86   23)
( 87   12) ( 88    6) ( 89   10) ( 90   15) ( 91    3)
(100    4) (101    9) (102   13) (103   30) (104  171)
(105   18) (106    8) (114    7) (115   20) (116   10)
(117    9) (118   23) (119   72) (120    7) (121    3)
(130    4) (131   20) (132  160) (133   74) (134   24)
(135    9) (144    5) (145    7) (146   22) (147  202)
(148   44) (149   33) (150    5) (151    3) (158    6)
(159    5) (160   40) (161   34) (162    6) (163    8)
(164    4) (173    4) (174   73) (175   11) (176   16)
(177   14) (178    6) (188    3) (189   18) (190    4)
(191   33) (192  110) (193   21) (194    9) (204    3)
(205   25) (206   63) (207   25) (208    8) (218    4)
(219   14) (220  271) (221   67) (222   34) (223    6)
(232    3) (233    5) (234    9) (235   14) (236    9)
(237    3) (246    3) (247    5) (248   35) (249   14)
(250    8) (251    6) (262    4) (263    4) (264   17)
(265    5) (266    3) (267    6) (277   23) (278    6)
(279   11) (280    4) (281    3) (293    3) (294    7)
(295   22) (296    5) (308    4) (322    3) (323    8)
(324    3) (335    3) (336   17) (337   13) (338    6)
(366   21) (367  109) (368   36) (369   18) (370    4)
(383    3)
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NAME:13C_3185.4_1313EC07_
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:318001-11-1
RI:3185
RT:18.659
NUM PEAKS:  138
( 70    5) ( 71    5) ( 72   17) ( 73 1000) ( 74   94)
( 75   99) ( 76    6) ( 77    6) ( 84    3) ( 85    8)
( 86   36) ( 87   13) ( 88    4) ( 89    9) ( 90    6)
( 98    4) (100    3) (101    6) (102    9) (103   22)
(104   86) (105    9) (106    3) (114    5) (115   35)
(116   17) (117    8) (118   13) (119   32) (130    6)
(131   21) (132  133) (133   73) (134   17) (135   12)
(137    4) (144    6) (145    8) (146   22) (147  233)
(148   39) (149   28) (151    5) (158    8) (159    5)
(160   37) (161   19) (162    3) (173    5) (174   48)
(175   10) (176    9) (177    7) (178    7) (181    6)
(186    3) (187    3) (188    8) (189   16) (190    4)
(191   31) (192   36) (193   13) (195    6) (203    3)
(204    4) (205   10) (206   54) (207   27) (208    7)
(209    4) (210    3) (211   52) (212   11) (213    4)
(218    5) (219    3) (220   98) (221   30) (222   11)
(225    8) (227   19) (232    3) (233    5) (234    6)
(235    9) (236    4) (243   11) (245    3) (246    4)
(247   23) (248   32) (249   12) (250    5) (255    5)
(261    4) (262    5) (275    3) (276   30) (277  187)
(278   34) (279   16) (283    4) (285    7) (294    7)
(298    7) (299   89) (300   24) (301   13) (308    6)
(309    3) (313    4) (314   13) (315  194) (316   52)
(317   26) (318    4) (322    3) (323    4) (338    7)
(359    5) (366    3) (367   22) (368    6) (373    7)
(386   13) (387   70) (388   25) (389   15) (390    3)
(428    4) (429   16) (430    5) (431    3) (518    7)
(519   21) (520    9) (521    6)

NAME:13C_2718.2_1313EC07_
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:272002-11-1
RI:2718
RT:16.522
NUM PEAKS:  159
( 70    5) ( 71    7) ( 72   16) ( 73 1000) ( 74   91)
( 75   76) ( 76    3) ( 77   15) ( 79    3) ( 84    3)
( 85    8) ( 86   13) ( 87    7) ( 88    4) ( 89   26)
( 90    6) ( 91    6) ( 98    3) ( 99    3) (100    3)
(101    7) (102   12) (103   41) (104    9) (105   11)
(106    3) (107    4) (114    3) (115   14) (116   12)
(117    8) (118   15) (119   12) (121    6) (129    4)
(130    5) (131   18) (132   79) (133   73) (134   15)
(135   21) (136    3) (137   11) (144    6) (145   26)
(146    9) (147  119) (148   19) (149   15) (150    3)
(151    9) (158    4) (159    4) (160    5) (161    7)
(163    5) (165    4) (167    3) (173    5) (174    5)
(175    4) (176   28) (177    6) (179    3) (181   13)
(182    3) (183    5) (186    8) (187    4) (188    3)
(189    4) (190    3) (191   14) (192   16) (193   16)
(194    4) (195   14) (196    3) (197    4) (202    6)
(203    4) (204    3) (205    4) (206   24) (207   23)
(208    6) (209    6) (210    3) (211   74) (212   12)
(213    7) (218    4) (219    5) (220   88) (221   18)
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(222    8) (225   30) (226    7) (227   19) (228    3)
(233    4) (234    5) (237    9) (238    3) (241    3)
(242    4) (243    4) (248    3) (255    5) (268    3)
(269    3) (274    5) (275    3) (276    4) (283    7)
(284    4) (285    8) (298   17) (299  157) (300   47)
(301   24) (302    5) (306    3) (313    4) (314   19)
(315  153) (316   44) (317   23) (318    4) (329    4)
(343    6) (355    3) (356   14) (357    7) (358    8)
(359   25) (360    8) (361    4) (371    3) (372    5)
(373    6) (374    3) (385    4) (386   28) (387  100)
(388   41) (389   22) (390    5) (416    6) (417   16)
(418    6) (419    3) (450    3) (451    6) (452    3)
(461    4) (462   12) (463    6) (464    3)

NAME:13C_2724.4_1313EC07_
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:272001-11-1
RI:2724
RT:16.554
NUM PEAKS:  143
( 70    6) ( 71    6) ( 72   17) ( 73 1000) ( 74   92)
( 75   75) ( 76    4) ( 77   15) ( 85    9) ( 86   11)
( 87    6) ( 88    3) ( 89   36) ( 90    7) ( 91    7)
( 98    3) ( 99    3) (100    3) (101    8) (102   12)
(103   44) (104   15) (105   13) (106    3) (107    5)
(114    3) (115   14) (116   10) (117    9) (118   14)
(119   13) (120    3) (121    6) (123    3) (129    4)
(130    5) (131   18) (132   94) (133   74) (134   17)
(135   22) (136    3) (137   12) (144    5) (145   30)
(146    9) (147  109) (148   17) (149   14) (151   10)
(158    3) (159    4) (160    4) (161    8) (163    6)
(165    4) (167    3) (173    4) (175    4) (176   34)
(177    7) (179    3) (181   14) (182    3) (183    4)
(186    4) (189    4) (190    3) (191   12) (193   13)
(194    3) (195   15) (196    3) (197    4) (202    4)
(203    3) (205    4) (207   24) (208    6) (209    6)
(210    4) (211   71) (212   11) (213    7) (218    4)
(219    6) (220   91) (221   17) (222    8) (225   39)
(226    8) (227   18) (228    3) (233    3) (234    6)
(237   10) (238    3) (241    4) (242    4) (243    3)
(255    4) (268    4) (269    4) (274    4) (277    3)
(283    8) (284    4) (285    8) (298   18) (299  171)
(300   50) (301   25) (302    5) (313    5) (314   18)
(315  149) (316   42) (317   22) (318    4) (329    4)
(343    6) (355    3) (356   11) (357    6) (358    8)
(359   25) (360    8) (361    4) (372    3) (373    6)
(374    3) (385    5) (386   34) (387  121) (388   49)
(389   26) (390    7) (417    5) (451    5) (461    3)
(462    9) (463    4) (550    3)

NAME:13C_2562.2_1313EC07_
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:256001-11-1
RI:2562
RT:15.693
NUM PEAKS:  136
( 71    8) ( 72   18) ( 73 1000) ( 74   92) ( 75   88)
( 76    8) ( 77   10) ( 84    3) ( 85   21) ( 86    7)
( 87    9) ( 88    5) ( 89   39) ( 90   13) ( 91    6)
( 98    3) (100    4) (101    9) (102   12) (103   40)
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(104   98) (105   20) (106    6) (107    3) (114    3)
(115   10) (116   18) (117    9) (118   15) (119   24)
(120    5) (121    5) (129    3) (130    5) (131   20)
(132   72) (133   62) (134   30) (135   16) (136    3)
(137    5) (144    3) (145   10) (146   11) (147  133)
(148   24) (150    5) (151    5) (158    4) (160    6)
(161   29) (162    6) (163    6) (164    3) (165    3)
(173   11) (174    7) (175    4) (176   12) (177    5)
(181    6) (183    3) (188    3) (189    4) (190    3)
(191   15) (192   15) (193   10) (194    3) (195    6)
(203    5) (204    5) (205    4) (206   25) (207   17)
(208    5) (209    3) (211   37) (212    6) (213    3)
(218    4) (219    6) (220   38) (221    9) (222    6)
(225   11) (227    8) (232    4) (233    4) (234    3)
(235    4) (243    3) (247    3) (248    3) (249    3)
(250    3) (251    6) (255    5) (264    5) (265   10)
(266    5) (283    5) (284    3) (285    5) (298   10)
(299   89) (300   28) (301   12) (313    3) (314    7)
(315   41) (316   12) (317    6) (329    4) (331    3)
(336    4) (343    6) (344    3) (358    8) (359   34)
(360   11) (361    5) (372    3) (373    4) (385    4)
(386   33) (387  116) (388   51) (389   24) (390    6)
(403    3) (474    6) (475   16) (476    8) (477    5)
(478    3)

NAME:13C_2579.9_1313EC07_
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:258001-11-1
RI:2580
RT:15.787
NUM PEAKS:  335
( 70   29) ( 71   30) ( 72  214) ( 73 1000) ( 74  332)
( 75  309) ( 76   39) ( 77   31) ( 78    6) ( 79    8)
( 80    6) ( 82    7) ( 83   27) ( 84   13) ( 85   68)
( 86   31) ( 87  155) ( 88   55) ( 89  137) ( 90   45)
( 91   15) ( 92    8) ( 93    7) ( 94    6) ( 96    7)
( 98   32) ( 99   11) (100   49) (101   31) (102  121)
(103  171) (104  352) (105   49) (106   19) (109    6)
(111    8) (113   11) (114    8) (115   36) (116   22)
(117   59) (118  109) (119  135) (120   22) (121    6)
(122    5) (124    6) (125    7) (126    3) (128   15)
(129   12) (130   49) (131   51) (132  492) (133  179)
(134  136) (135   31) (136    5) (137    4) (138    7)
(139    7) (141    7) (142    6) (143   13) (144   12)
(145   41) (146   19) (147  420) (148  106) (149   73)
(150   24) (151   10) (152    7) (153    6) (154    3)
(156   10) (157    6) (158   11) (159   10) (160   24)
(161   17) (162   16) (163   15) (164    9) (165    8)
(167    5) (168    6) (169    5) (170    5) (171    4)
(172    8) (173    8) (174    6) (175   11) (176    8)
(177   24) (178   13) (179    6) (180    3) (181    4)
(183    5) (184    3) (185    4) (186    4) (187    6)
(188    6) (190    8) (191    9) (192   22) (193   16)
(194    6) (195    6) (196    6) (197    4) (198    5)
(199    4) (200    3) (201    3) (202    8) (203    4)
(204    3) (205    9) (206  147) (207  139) (208   29)
(209   13) (210    5) (221    9) (222   35) (223    9)
(224   11) (226    7) (229    5) (231    4) (232    3)
(233    3) (234   12) (235   15) (236    5) (237    7)
(238    7) (239    5) (240   11) (241    6) (242    7)
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(243    4) (244    3) (245    4) (246    8) (247    4)
(249    4) (250    4) (252   20) (253   43) (254    8)
(256    4) (260    4) (262    4) (265    5) (266    7)
(267   31) (268   15) (269    7) (270    5) (271    4)
(272    4) (275    3) (279    6) (280    9) (281    5)
(282    8) (283    6) (284    3) (285    4) (290    3)
(292    7) (294    4) (295    4) (296    8) (297   24)
(298   11) (300    5) (301    4) (302    4) (303    3)
(305    4) (306    5) (307    3) (309    9) (310    7)
(311    7) (312    6) (313    3) (314    6) (315    5)
(316    8) (317    5) (318    4) (319    3) (320    4)
(321    3) (322    5) (325   11) (326   10) (327   14)
(328    3) (329    4) (331    7) (332    6) (334    5)
(337    5) (338    4) (340    7) (344    6) (345    6)
(347    5) (348    6) (353    3) (355    8) (356    6)
(357    5) (360    4) (361    7) (371    6) (373    5)
(374    4) (375    5) (378    4) (381    7) (382    5)
(383    4) (384    5) (385   15) (386   27) (387   88)
(388   29) (389    9) (390    4) (391    4) (395    6)
(396    6) (397    4) (398    7) (399    7) (400    8)
(401   15) (402    7) (403   10) (406    4) (408    4)
(409    3) (410    5) (412    4) (415    7) (419    5)
(420    5) (422    3) (423    5) (424    5) (429    4)
(430    3) (431    7) (432    4) (438    4) (439    6)
(440    4) (441    3) (443    4) (444    4) (446    4)
(447    4) (453    3) (454    4) (455    5) (456    5)
(458    5) (459    6) (460    4) (461    4) (462    5)
(463    5) (464    6) (465    5) (466    3) (467    3)
(472    5) (473    6) (474    4) (475    9) (476   12)
(477    9) (478    6) (479    4) (483    4) (484    4)
(485    6) (486    4) (488    5) (491    4) (492    6)
(493    6) (496    3) (497    4) (502    4) (503    5)
(506    5) (508    3) (509    5) (512    4) (517    3)
(522    7) (525    4) (526    4) (528    5) (531    4)
(536    3) (539    3) (540    3) (541    7) (542    3)
(544    5) (546    4) (547    4) (548    3) (550    3)
(551    3) (552    4) (555    3) (558    5) (561    4)
(564    3) (572    4) (584    3) (590    3) (591    3)

NAME:13C_2390.1_1313EC07_
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:239001-11-1
RI:2390
RT:14.779
NUM PEAKS:  108
( 70    5) ( 71    9) ( 73 1000) ( 74   90) ( 75  102)
( 76    7) ( 77   11) ( 84    3) ( 85    8) ( 86   16)
( 87    8) ( 88    4) ( 89    7) ( 90    4) ( 99    3)
(100    3) (101    5) (102    9) (103   28) (104   29)
(105   10) (107    3) (113    3) (114    5) (115   15)
(116   15) (117    8) (118   14) (119   15) (121    3)
(130    4) (131   22) (132  113) (133   65) (134   13)
(135   15) (137    5) (145    5) (146   13) (147  149)
(148   26) (149   22) (150    3) (151    5) (160   10)
(161    7) (164    3) (174   10) (175    3) (176    3)
(177    3) (181    6) (189    5) (191   26) (192   37)
(193   16) (194    4) (195    6) (205    7) (206  163)
(207   40) (208   15) (209    3) (211   41) (212    7)
(213    4) (219    3) (220   45) (221   11) (222    5)
(225    9) (226    3) (227    8) (235    3) (243    3)
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(247 5) (248 6) (249 3) (255 5) (271 4)
(276 6) (277 13) (278 3) (283 4) (285 5)
(298 11) (299 98) (300 28) (301 13) (302 3)
(308 4) (314 6) (315 28) (316 8) (317 4)
(351 6) (358 6) (359 26) (360 8) (361 4)
(372 5) (373 17) (374 6) (386 24) (387 82)
(388 35) (389 18) (390 5)

NAME:13C_2347.2_1313EC07_Glucose-6-phosphate methoxyamine (BP) (6TMS)
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:235002-11-1
RI:2347
RT:14.551
NUM PEAKS: 96
(70 5) (71 10) (72 16) (73 1000) (74 89)
(75 79) (76 5) (85 8) (86 5) (87 8)
(88 3) (89 49) (90 9) (101 13) (102 12)
(104 43) (107 3) (115 8) (116 11) (118 17)
(119 12) (120 3) (121 4) (131 17) (132 73)
(133 70) (134 18) (135 15) (137 6) (145 4)
(146 9) (147 114) (148 19) (149 13) (151 6)
(158 3) (160 4) (161 33) (162 40) (163 15)
(164 3) (173 3) (174 5) (181 7) (192 7)
(193 10) (194 3) (195 8) (197 3) (207 15)
(208 3) (209 3) (211 46) (212 8) (213 4)
(220 30) (225 13) (226 3) (227 10) (233 4)
(234 5) (235 5) (243 4) (248 3) (251 6)
(255 5) (283 4) (285 4) (298 12) (299 105)
(300 32) (301 15) (302 3) (313 3) (314 8)
(315 46) (316 14) (317 7) (331 4) (343 5)
(344 3) (358 8) (359 35) (360 11) (361 5)
(373 4) (385 3) (386 32) (387 116) (388 49)
(389 26) (390 7) (474 4) (475 12) (476 6)
(477 3)

NAME:13C_2313.4_1313EC07_Galactose-6-phosphate methoxyamine (6TMS)
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:232001-11-1
RI:2313
RT:14.372
NUM PEAKS: 108
(70 5) (71 5) (72 17) (73 1000) (74 90)
(75 91) (76 5) (77 9) (86 9) (87 11)
(88 5) (89 37) (90 8) (91 4) (100 3)
(101 14) (102 12) (103 48) (105 23) (106 4)
(107 3) (115 10) (116 17) (117 9) (118 16)
(119 14) (121 4) (129 3) (130 6) (131 20)
(132 72) (133 66) (134 16) (135 15) (137 6)
(144 4) (145 7) (146 11) (147 144) (148 24)
(149 16) (151 6) (159 3) (160 5) (161 30)
(162 61) (163 14) (164 4) (173 4) (174 5)
(175 3) (176 5) (177 4) (181 7) (189 3)
(190 3) (191 14) (192 9) (193 11) (195 8)
(203 3) (204 3) (205 4) (206 12) (207 19)
(208 5) (209 3) (211 42) (212 7) (213 4)
(218 6) (219 8) (225 12) (226 3) (227 10)
(232 3) (233 4) (234 6) (235 5) (248 3)
(249 3) (251 4) (255 5) (283 4) (285 4)
(298 9) (299 89) (300 26) (301 13) (302 3)
(331 6) (336 6) (343 6) (358 7) (359 32)

(360 10) (361 5) (373 3) (385 3) (386 27)
(387 101) (388 42) (389 23) (390 6) (474 4)
(475 11) (476 5) (477 3)

NAME:13C_2311.9_1313EC07_Fructose-6-phosphate methoxyamine (6TMS)
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:232002-11-1
RI:2312
RT:14.363
NUM PEAKS: 135
(70 4) (71 8) (72 12) (73 1000) (74 93)
(75 16) (77 5) (85 27) (86 5) (89 36)
(90 15) (91 6) (98 3) (101 4) (102 5)
(103 37) (104 122) (105 12) (106 7) (114 3)
(115 7) (116 18) (117 8) (118 12) (119 33)
(120 7) (129 4) (130 4) (131 19) (132 87)
(133 47) (134 30) (135 14) (137 6) (142 3)
(145 9) (146 5) (147 163) (148 27) (149 18)
(150 3) (151 5) (158 3) (159 4) (160 6)
(173 9) (174 3) (175 3) (176 7) (177 3)
(181 8) (183 3) (186 4) (188 3) (189 4)
(191 6) (192 11) (193 9) (195 8) (203 4)
(204 3) (205 3) (206 14) (207 16) (208 6)
(209 3) (211 52) (212 10) (213 5) (217 3)
(218 3) (219 9) (220 177) (221 39) (222 17)
(223 4) (225 15) (226 4) (227 21) (228 4)
(233 3) (237 3) (248 4) (249 3) (255 5)
(260 3) (261 4) (262 3) (263 3) (264 5)
(265 10) (266 4) (267 3) (274 3) (276 3)
(283 3) (285 5) (297 3) (298 10) (299 86)
(300 31) (301 15) (302 4) (306 3) (307 3)
(308 3) (309 3) (313 3) (314 28) (315 274)
(316 79) (317 41) (318 8) (319 3) (322 3)
(323 3) (329 4) (343 6) (344 3) (345 3)
(358 5) (359 19) (360 7) (361 4) (362 3)
(372 3) (373 7) (374 5) (402 4) (403 11)
(404 5) (461 12) (462 30) (463 14) (464 6)

NAME:13C_2257.9_1313EC07_
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:226001-11-1
RI:2258
RT:14.076
NUM PEAKS: 138
(70 7) (71 10) (72 31) (73 1000) (74 113)
(75 105) (76 8) (84 5) (85 15) (86 9)
(87 25) (88 20) (89 245) (90 21) (98 3)
(99 3) (100 9) (101 16) (102 13) (103 20)
(104 187) (105 17) (106 5) (113 4) (114 5)
(115 9) (116 12) (118 12) (119 53) (130 8)
(131 25) (132 24) (133 39) (134 10) (142 4)
(144 6) (145 19) (146 20) (147 228) (148 44)
(149 22) (156 3) (157 5) (158 4) (159 7)
(160 8) (161 10) (163 5) (171 3) (172 6)
(173 14) (174 5) (175 8) (176 12) (177 7)
(178 5) (179 26) (180 3) (186 5) (187 6)
(188 9) (189 7) (190 3) (191 19) (192 16)
(193 7) (202 4) (203 5) (204 6) (205 5)
(207 25) (208 28) (209 4) (214 3) (218 3)
(219 7) (220 78) (221 20) (222 6) (232 4)

(233 12) (246 3) (247 8) (248 3) (251 3)
(259 3) (260 4) (261 7) (262 6) (263 4)
(265 6) (266 3) (274 3) (275 4) (276 6)
(277 3) (278 3) (279 7) (280 3) (291 3)
(292 3) (293 3) (294 4) (296 3) (304 3)
(305 3) (306 3) (307 4) (309 3) (310 7)
(334 5) (335 14) (336 7) (337 3) (350 3)
(351 6) (352 5) (378 4) (379 3) (380 8)
(381 9) (382 23) (383 7) (410 3) (411 4)
(441 3) (442 4) (452 3) (453 8) (454 4)
(468 4) (483 4) (484 3) (558 5) (559 3)
(560 3) (561 6) (562 3)

NAME:13C_2294.1_1313EC07_
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:230001-11-1
RI:2294
RT:14.269
NUM PEAKS: 188
(70 7) (71 5) (73 758) (74 78) (75 66)
(80 4) (82 5) (86 7) (90 24) (94 9)
(97 6) (99 15) (103 62) (104 320) (105 34)
(107 9) (110 12) (112 9) (113 4) (115 21)
(116 18) (117 21) (118 21) (125 5) (130 14)
(132 78) (133 56) (135 12) (136 7) (141 5)
(143 11) (144 8) (146 31) (148 24) (149 20)
(152 7) (153 5) (156 8) (157 24) (161 11)
(162 11) (164 12) (166 8) (168 13) (172 7)
(173 6) (174 15) (176 7) (179 12) (183 6)
(184 9) (185 9) (187 11) (188 6) (191 31)
(192 54) (193 9) (195 14) (196 6) (197 9)
(198 8) (199 8) (200 9) (204 8) (205 40)
(206 1000) (207 122) (208 63) (213 6) (214 6)
(215 12) (217 22) (218 7) (220 50) (221 23)
(222 41) (223 8) (232 6) (234 9) (236 15)
(237 15) (243 7) (244 13) (246 5) (247 7)
(252 7) (253 8) (257 6) (259 12) (260 15)
(263 14) (264 10) (268 12) (269 16) (271 10)
(272 17) (278 6) (292 10) (302 6) (308 7)
(309 7) (317 14) (323 10) (324 10) (326 10)
(330 7) (332 12) (333 6) (339 15) (340 15)
(341 39) (343 12) (345 9) (346 8) (353 12)
(364 14) (365 13) (366 12) (367 20) (368 9)
(371 12) (376 14) (378 12) (379 13) (383 13)
(384 10) (389 9) (390 5) (391 12) (394 8)
(395 8) (402 18) (408 9) (410 10) (411 7)
(415 7) (421 13) (426 8) (430 10) (443 13)
(447 24) (448 9) (449 10) (453 16) (454 12)
(458 9) (459 12) (461 11) (471 8) (477 9)
(480 18) (483 6) (484 13) (488 10) (489 8)
(491 9) (493 13) (494 8) (499 12) (502 10)
(503 15) (504 7) (505 8) (509 12) (510 12)
(513 18) (514 14) (515 17) (524 8) (528 12)
(529 9) (532 8) (533 13) (548 14) (549 16)
(553 7) (555 16) (559 5) (560 6) (563 7)
(566 7) (569 12) (571 13) (575 7) (578 4)
(580 6) (590 7) (591 8)

NAME:13C_2285.3_1313EC07_
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:228001-11-1
RI:2285
RT:14.222
NUM PEAKS: 106
(71 7) (72 20) (73 1000) (74 95) (75 145)
(76 9) (77 5) (85 6) (86 9) (87 12)
(88 4) (89 39) (90 15) (100 4) (101 17)
(102 15) (103 51) (104 36) (105 26) (106 3)
(116 14) (117 10) (118 133) (119 330) (120 29)
(121 13) (130 5) (131 16) (132 62) (133 44)
(134 15) (135 5) (144 4) (145 9) (146 25)
(147 132) (148 25) (149 18) (160 8) (161 98)
(162 120) (163 60) (164 10) (165 3) (173 5)
(174 5) (176 6) (177 6) (190 3) (191 16)
(192 9) (193 11) (203 3) (204 4) (206 6)
(207 9) (209 4) (215 3) (216 5) (218 6)
(219 10) (220 71) (221 20) (222 9) (233 4)
(234 8) (235 16) (236 7) (237 15) (238 3)
(248 5) (251 13) (252 3) (253 13) (262 5)
(263 3) (264 3) (265 4) (274 3) (278 4)
(280 5) (281 4) (294 4) (296 10) (297 82)
(298 16) (306 4) (307 3) (308 4) (309 3)
(310 4) (323 10) (324 4) (325 10) (326 3)
(327 3) (333 3) (334 4) (352 3) (368 3)
(412 6) (413 25) (414 9) (415 4) (441 3)
(513 3)

NAME:13C_1396.1_1313EC11_
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:140003-11-1
RI:1396
RT: 7.541
NUM PEAKS: 66
(70 5) (71 5) (72 21) (73 1000) (74 85)
(75 322) (76 10) (77 10) (84 1) (85 6)
(86 2) (91 12) (99 2) (103 50) (104 8)
(105 6) (110 1) (112 3) (117 13) (118 192)
(119 660) (120 59) (121 21) (126 2) (133 129)
(134 15) (135 14) (136 2) (137 2) (144 3)
(146 9) (149 115) (150 15) (161 2) (163 4)
(176 9) (177 11) (178 4) (191 2) (192 2)
(193 3) (200 4) (207 13) (208 3) (209 2)
(211 1) (216 2) (235 3) (236 10) (237 134)
(238 23) (239 9) (242 1) (249 1) (250 24)
(251 3) (252 3) (268 6) (288 1) (308 7)
(309 89) (310 24) (311 14) (312 2) (340 7)
(341 2)

NAME:13C_1475.5_1313EC07_Citramalic acid (3TMS)
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:148001-11-1
RI:1476
RT: 8.482
NUM PEAKS: 94
(70 7) (71 15) (72 90) (73 1000) (74 95)
(75 209) (76 21) (77 7) (86 3) (87 10)
(88 5) (89 37) (100 11) (101 9) (102 18)
(103 14) (104 5) (116 5) (117 16) (118 125)
(119 15) (120 4) (131 28) (132 10) (133 76)
(134 11) (135 10) (136 1) (137 1) (146 9)

```
(147  368) (148   69) (149   76) (150   10) (151    7)
(152    1) (160    4) (161   19) (162    2) (163   28)
(164    4) (165    2) (174    4) (175    5) (176    3)
(178    1) (190   22) (191    9) (192   21) (193    8)
(194    2) (206   31) (207   11) (208    3) (211    2)
(218    1) (219    8) (221   32) (222    7) (223    3)
(224    1) (227    2) (229    1) (234   26) (235   35)
(236   18) (237    5) (238    1) (247    1) (250    7)
(251  136) (252   23) (253   11) (254    1) (263    2)
(264   32) (265    5) (266    4) (280    3) (293    1)
(299    3) (301    1) (308    2) (309    4) (310    1)
(322    1) (324    1) (325   15) (326    6) (337    2)
(338    1) (353    1) (354   10) (355    3)
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NAME:13C_1735.8_1313EC07_Glycerol-2-phosphate (4TMS)
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:174002-11-1
RI:1736
RT: 10.586
NUM PEAKS: 421

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( 70    8) ( 71   21) ( 72   39) ( 73 1000) ( 74  110)
( 75  219) ( 76   14) ( 77   39) ( 78    3) ( 79   13)
( 80   14) ( 81   10) ( 82   19) ( 83   10) ( 84   26)
( 85   11) ( 86    1) ( 87  155) ( 88   35) ( 89   31)
( 90    8) ( 91   27) ( 92    8) ( 93    5) ( 94    7)
( 95    3) ( 96    4) ( 98   16) ( 99   11) (100   28)
(101   25) (102   49) (103  149) (105   26) (106   11)
(107   16) (108    3) (109   10) (111   10) (112   10)
(113   14) (114    6) (115   51) (116   20) (117   29)
(118   82) (121   25) (124   15) (127   24) (128   34)
(129   33) (130   24) (131   47) (132  136) (133   81)
(134   15) (135   20) (136    5) (137   14) (138    8)
(139    6) (141   49) (142   12) (144   12) (146   15)
(147  185) (148    5) (149   12) (151   24) (152   34)
(153   19) (154    4) (155   27) (156   19) (157   61)
(158    2) (159   23) (160   11) (162   13) (165    4)
(166   10) (167    2) (168    2) (169    2) (170    9)
(171    7) (172    7) (174    1) (175  435) (176   28)
(177   42) (178    5) (179   22) (180   95) (181   46)
(182   16) (183   16) (184   15) (185   15) (186   19)
(187    4) (189   25) (190   73) (191    3) (192   14)
(193   23) (194    8) (195   12) (196   14) (197   18)
(198   29) (199    8) (201   15) (202    5) (203   25)
(205    1) (210    3) (211  227) (212   41) (213   31)
(214    9) (215    6) (216    9) (217   18) (218   21)
(223   14) (224    3) (225    8) (227   38) (228    2)
(229   13) (230    1) (231   76) (232   24) (234    2)
(235    2) (236    5) (238   14) (239    4) (240    6)
(242   20) (243  294) (244   54) (245   38) (246   11)
(247    3) (249   11) (251    1) (252    9) (253    9)
(255    7) (256    6) (257    9) (258    3) (259   17)
(260   16) (261    8) (263    5) (265   10) (266    3)
(267    9) (268   14) (269   83) (270   22) (271    8)
(272    3) (273    3) (274   12) (275   14) (276   12)
(277   13) (280    9) (282    6) (283   26) (284   17)
(285   32) (286   12) (287   12) (288    6) (291    4)
(294    8) (295    8) (296    7) (297    5) (298   19)
(299  173) (300   60) (301   36) (302    8) (303    5)
(304    6) (306    1) (308   32) (309   24) (311    3)
(312    7) (313    9) (314   14) (315   36) (316   14)
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(318    7) (319    6) (320    9) (321   25) (322    4)
(326    8) (329   12) (330    3) (331   12) (332    9)
(333    8) (334    7) (337    9) (338    9) (339    9)
(340    9) (341    4) (343    8) (344    2) (345    5)
(346    9) (347   12) (348   22) (349    8) (351   13)
(352    9) (353    8) (355    8) (356    7) (357    9)
(358    5) (359    8) (360   10) (361    5) (362    5)
(363   12) (364    3) (365    4) (370   11) (371    3)
(372   13) (373   21) (374   15) (375   21) (376   13)
(377   12) (378   18) (379    3) (380   15) (381    5)
(384    5) (385   15) (386    7) (387    6) (388    7)
(389   27) (390   18) (391    4) (392   10) (393    9)
(394   10) (395    9) (396   12) (397    6) (398    3)
(399   14) (400    9) (401   17) (402    1) (403    6)
(404   13) (405    6) (407    7) (408    3) (409    4)
(411   12) (414    2) (415    7) (416   15) (417   11)
(418    8) (419    4) (420    7) (421    2) (422    3)
(423   15) (424    4) (426   13) (427    2) (429    5)
(430    2) (431    1) (432    4) (433    1) (435    3)
(436   15) (437    7) (439   13) (440   15) (441    1)
(442    5) (443    2) (444    3) (446    6) (447    6)
(448   22) (449   12) (450    5) (451    6) (452    7)
(453    4) (454   10) (455   12) (457    2) (459   12)
(460   12) (461   11) (463   10) (466    6) (467    9)
(470   15) (471   12) (472    3) (473    9) (475   14)
(476   10) (478    1) (479    6) (480   10) (481    6)
(482    8) (483    1) (484    9) (485   13) (486    2)
(487    5) (488    6) (489    4) (491   10) (492    6)
(493   10) (494    8) (495    9) (496    5) (498    8)
(499    9) (500    6) (501    8) (502    2) (503    7)
(504    9) (505    2) (507    9) (508    5) (509   23)
(510    9) (512    7) (513    3) (514    2) (516   11)
(517    9) (518    7) (519    8) (520    6) (521    5)
(522   11) (523    2) (524   10) (525    9) (527    5)
(528   18) (529   13) (530   15) (531    3) (532    4)
(534    2) (535   11) (536    6) (538    5) (539    2)
(540    5) (541    3) (542    6) (543   12) (544    6)
(546    5) (550   11) (551    8) (552   11) (554    3)
(555    4) (557    1) (558    9) (561   10) (562    4)
(563    6) (564    1) (565    7) (566    9) (569    1)
(570    3) (571    2) (572   11) (573    9) (574    3)
(575    1) (576    1) (578    2) (581    3) (582    1)
(583    2) (584    9) (587    1) (588    8) (590    1)
(591    3) (592    2) (594    3) (595    1) (596    2)
(597    3)

NAME:13C_1755.8_1313EC07_
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:176003-11-1
RI:1756
RT: 10.758
NUM PEAKS:  124
( 70   30) ( 71   81) ( 72   51) ( 73 1000) ( 79   12)
( 80    5) ( 81    5) ( 84   11) ( 85   57) ( 86   17)
( 87   45) ( 91    4) ( 92    3) ( 93    6) ( 94    3)
( 97   10) ( 98    3) ( 99   39) (101  125) (102   20)
(103   15) (108    2) (109    2) (112    5) (113   14)
(114    5) (115   26) (117   20) (121    1) (122    1)
(125    2) (126    7) (127   10) (130    4) (131   56)
(133   62) (134    9) (135    5) (140    2) (142    5)
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(143 18) (147 245) (148 47) (149 22) (156 2)
(157 4) (158 16) (159 21) (161 7) (170 3)
(171 10) (174 12) (175 50) (176 9) (184 6)
(185 7) (186 5) (187 7) (199 3) (200 9)
(201 4) (206 19) (214 5) (216 5) (217 16)
(230 5) (242 4) (243 15) (244 6) (245 4)
(246 4) (250 1) (256 11) (257 69) (258 282)
(259 63) (260 23) (261 4) (262 3) (272 2)
(273 9) (274 45) (275 9) (276 4) (287 9)
(288 4) (289 3) (290 3) (291 1) (301 2)
(308 1) (309 1) (315 1) (317 3) (331 6)
(332 6) (333 8) (334 5) (337 2) (347 3)
(360 5) (361 21) (362 79) (363 23) (364 10)
(369 1) (370 1) (376 7) (377 9) (378 3)
(387 1) (388 1) (418 1) (443 2) (455 1)
(466 1) (489 2) (506 1) (513 1) (558 1)
(573 1) (584 1) (589 1) (592 1)

NAME:13C_1761.5_1313EC07_
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:176004-11-1
RI:1762
RT: 10.791
NUM PEAKS: 88
(70 13) (73 1000) (83 4) (89 102) (90 22)
(91 5) (98 5) (99 44) (103 42) (104 95)
(105 41) (106 5) (111 1) (119 73) (120 7)
(121 2) (127 5) (128 8) (129 28) (133 68)
(134 35) (135 8) (136 1) (143 8) (144 10)
(145 214) (147 114) (149 14) (156 2) (157 4)
(163 11) (164 2) (170 1) (171 3) (172 12)
(173 26) (185 4) (186 5) (187 4) (188 13)
(189 60) (201 4) (202 6) (203 19) (205 20)
(206 8) (207 36) (208 5) (209 2) (217 7)
(231 7) (232 2) (234 24) (235 500) (236 57)
(237 19) (238 1) (247 3) (261 1) (271 1)
(276 2) (277 5) (278 1) (279 2) (290 2)
(291 2) (292 2) (305 1) (306 1) (307 1)
(309 1) (310 6) (311 1) (319 1) (320 3)
(321 18) (322 4) (323 1) (337 4) (338 3)
(339 1) (348 1) (410 2) (411 7) (412 2)
(413 1) (426 1) (427 2)

NAME:13C_1796.3_1313EC07_
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:180001-11-1
RI:1796
RT: 11.063
NUM PEAKS: 145
(70 21) (71 20) (72 35) (73 1000) (74 95)
(75 235) (76 17) (77 12) (84 8) (85 17)
(86 11) (87 38) (88 133) (89 79) (90 19)
(91 6) (92 2) (98 9) (99 101) (100 16)
(101 23) (102 17) (103 68) (104 117) (105 88)
(106 11) (107 3) (113 4) (114 4) (115 19)
(116 13) (117 15) (118 44) (119 71) (120 8)
(121 2) (126 1) (127 7) (128 12) (129 11)
(130 10) (131 32) (132 71) (133 85) (134 27)
(135 7) (136 1) (142 2) (143 5) (144 12)
(145 22) (146 15) (147 142) (148 32) (149 27)

(150 3) (151 3) (156 3) (157 4) (158 6)
(159 14) (160 58) (161 14) (162 52) (163 20)
(164 4) (166 1) (172 8) (173 18) (174 6)
(177 11) (178 18) (179 2) (183 4) (187 3)
(188 2) (189 6) (191 36) (192 21) (199 2)
(200 4) (202 6) (203 80) (204 13) (205 29)
(206 18) (207 43) (208 8) (209 3) (217 4)
(218 6) (219 3) (220 47) (221 9) (222 39)
(223 4) (224 1) (230 1) (231 7) (232 2)
(233 5) (234 11) (235 109) (236 13) (237 4)
(240 1) (246 2) (247 2) (248 7) (249 1)
(263 6) (264 1) (275 3) (276 2) (277 7)
(278 2) (279 2) (281 3) (282 3) (290 2)
(291 1) (296 1) (305 2) (306 2) (308 1)
(309 2) (310 11) (311 3) (312 1) (320 3)
(321 20) (322 5) (323 2) (324 2) (325 9)
(326 1) (336 1) (337 5) (338 5) (351 1)
(352 2) (381 1) (411 3) (412 1) (427 1)

NAME:13C_3379.6_1313EC07_Lanosta-8,24-dien-3-beta-ol (1TMS)
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:338001-11-1
RI:3380
RT:19.444
NUM PEAKS: 303
(70 50) (71 29) (72 235) (73 810) (74 1000)
(75 516) (76 61) (77 21) (78 5) (79 6)
(80 8) (81 9) (82 17) (83 91) (84 31)
(85 144) (86 29) (87 250) (88 41) (89 135)
(90 10) (91 23) (92 5) (93 5) (94 6)
(95 8) (96 14) (97 19) (98 182) (99 28)
(100 176) (101 38) (102 289) (103 33) (104 53)
(105 8) (106 5) (107 5) (109 7) (110 9)
(111 24) (112 25) (113 199) (114 28) (115 176)
(116 40) (117 303) (118 22) (119 49) (120 15)
(121 5) (122 4) (123 8) (124 50) (125 21)
(126 68) (127 27) (128 189) (129 33) (130 157)
(131 37) (132 342) (133 32) (134 25) (135 8)
(136 7) (137 24) (138 57) (139 68) (140 31)
(141 118) (142 24) (143 124) (144 28) (145 133)
(146 17) (147 67) (148 13) (149 10) (150 7)
(151 8) (152 39) (153 36) (154 74) (155 35)
(156 130) (157 28) (158 118) (159 20) (160 77)
(161 8) (162 40) (163 10) (164 16) (165 18)
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(176 8) (177 22) (178 17) (179 6) (180 11)
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(216 48) (217 14) (218 37) (219 8) (220 20)
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(229 41) (230 18) (231 55) (232 7) (233 18)
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(246 47) (247 6) (248 9) (249 3) (254 4)

(255 5) (256 5) (257 15) (258 20) (259 79)
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(406 3) (413 3) (414 3) (419 7) (420 19)
(421 53) (422 149) (423 29) (429 3) (433 3)
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(457 3) (461 3) (466 3) (471 3) (477 3)
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(528 36) (529 16) (530 4) (532 3) (535 3)
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NAME:13C_3079.3_1313EC07_
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:308001-11-1
RI:3079
RT:18.190
NUM PEAKS: 175
(70 12) (71 14) (72 40) (73 1000) (74 96)
(75 112) (76 8) (77 12) (83 5) (84 8)
(85 10) (86 23) (87 11) (88 6) (89 7)
(90 4) (91 4) (96 5) (97 3) (98 7)
(99 6) (100 11) (101 10) (102 22) (103 28)
(104 9) (105 7) (107 3) (111 6) (112 25)
(113 6) (114 5) (115 13) (116 15) (117 15)
(118 12) (119 13) (121 5) (123 3) (124 7)
(125 3) (126 4) (129 10) (130 6) (131 24)
(132 63) (133 82) (134 13) (135 21) (136 3)
(137 10) (138 4) (139 15) (140 71) (141 66)
(142 3) (143 3) (144 24) (145 15) (146 28)
(147 154) (148 26) (149 21) (150 3) (151 8)
(152 4) (153 6) (154 9) (155 7) (158 11)
(159 4) (160 5) (161 6) (162 3) (165 3)
(167 7) (168 6) (169 12) (170 34) (172 4)
(173 21) (174 418) (175 42) (176 41) (177 4)
(179 3) (180 3) (181 18) (182 7) (183 10)
(184 3) (189 6) (190 3) (191 10) (192 3)
(193 10) (194 4) (195 18) (196 9) (197 22)
(198 5) (199 4) (205 3) (206 3) (207 14)
(208 4) (209 5) (210 8) (211 114) (212 32)
(213 36) (214 5) (218 12) (219 5) (220 16)
(222 3) (223 4) (224 9) (225 20) (226 7)
(227 25) (228 6) (229 3) (233 7) (234 123)
(235 22) (236 10) (240 6) (241 17) (242 9)
(243 11) (247 13) (248 43) (249 10) (250 4)

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(255    7) (256    7) (257   15) (258    3) (262    9)
(263   65) (264   16) (265    6) (269    5) (270    7)
(271    7) (272   19) (273    3) (283    4) (284    3)
(285    8) (286    3) (298    8) (299   76) (300   24)
(301   12) (302    3) (312    4) (313    8) (314   25)
(315  214) (316   66) (317   30) (318    6) (329    3)
(373    3) (374    8) (385    3) (386   19) (387   11)
(388    6) (389    3) (403    5) (404   15) (405    3)

NAME:13C_2679.5_1313EC07_
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:268001-11-1
RI:2680
RT:16.316
NUM PEAKS:  157
( 70    8) ( 71    9) ( 72   23) ( 73 1000) ( 74   91)
( 75  106) ( 76    7) ( 77   14) ( 83    3) ( 84    4)
( 85    8) ( 86   11) ( 87    9) ( 88    3) ( 89   10)
( 90    6) ( 91    4) ( 98   10) ( 99    3) (100    3)
(101    6) (102    9) (103   24) (104   30) (105    9)
(106    3) (107    4) (113    5) (114    4) (115   21)
(116    9) (117    7) (118    7) (119   18) (121    5)
(129    5) (130    5) (131   17) (132   72) (133   69)
(134   13) (135   19) (136    3) (137    9) (139    4)
(140    4) (141   23) (144   16) (145    9) (146   21)
(147  156) (148   27) (149   23) (150    4) (151    9)
(158    3) (159    4) (160   12) (161   14) (162    3)
(163    3) (165    3) (174    9) (175    3) (176    3)
(177    3) (178    9) (179    4) (181   11) (182    3)
(183    4) (188    4) (189   11) (190    3) (191   12)
(192   16) (193   13) (194    3) (195   12) (196    3)
(197    4) (202    4) (203    4) (205    7) (206   28)
(207   27) (208    6) (209    5) (210    5) (211   72)
(212   12) (213    7) (217    3) (218   43) (219   15)
(220   33) (225   32) (226    9) (227   23) (228    4)
(233    9) (234   64) (235   14) (236    6) (242    5)
(243    6) (248    3) (255    3) (256    4) (260    3)
(262    8) (263    3) (269    3) (276    5) (277   12)
(278    3) (283    6) (284    4) (285   12) (286    4)
(298   16) (299  133) (300   42) (301   20) (302    5)
(313    5) (314   19) (315  147) (316   45) (317   22)
(318    4) (328    4) (329   20) (330    6) (331    4)
(343    3) (344    5) (351    3) (358    6) (359   11)
(360    4) (372    3) (373    5) (374    3) (375    5)
(386    5) (387   17) (388    8) (389    5) (429    3)
(445    3) (446   10) (447   20) (448    9) (449    5)
(450    3) (518    3)

NAME:13C_1924.2_1313EC07_Mannitol (6TMS)
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:193002-11-1
RI:1924
RT:12.015
NUM PEAKS:  125
( 72   11) ( 73 1000) ( 74   89) ( 75    7) ( 87   26)
( 89   67) ( 90   32) ( 91    3) (100    6) (101   27)
(102   14) (103   27) (104  265) (105   45) (106   12)
(114    2) (115    4) (116    8) (117    8) (118    8)
(119  121) (120   13) (121    4) (128    1) (129    3)
(130    6) (131   42) (132  221) (133   87) (134   55)
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(135 9) (136 1) (144 1) (145 4) (146 17)
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(164 12) (173 4) (174 9) (175 2) (176 6)
(177 12) (178 8) (179 1) (184 1) (189 1)
(190 9) (191 50) (193 2) (198 2) (202 2)
(204 5) (205 3) (206 8) (207 234) (208 46)
(209 21) (210 1) (219 10) (220 95) (221 22)
(222 10) (232 2) (233 44) (234 10) (235 41)
(236 11) (237 17) (238 3) (239 1) (246 4)
(247 2) (248 7) (249 6) (250 4) (251 3)
(252 1) (264 3) (265 2) (266 2) (274 8)
(275 3) (276 1) (278 9) (279 14) (280 6)
(281 1) (285 1) (291 1) (294 14) (295 6)
(296 2) (306 2) (307 2) (308 2) (309 5)
(310 5) (311 4) (312 1) (321 1) (322 16)
(323 206) (324 72) (325 33) (326 6) (340 2)
(352 2) (353 1) (364 1) (369 1) (380 1)
(381 4) (382 2) (383 1) (454 1) (470 1)

NAME:13C_1546.0_1313EC07_
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:154001-11-1
RI:1546
RT:9.114
NUM PEAKS: 256
(70 14) (72 42) (73 1000) (74 277) (90 19)
(103 90) (104 108) (112 4) (116 94) (119 112)
(132 128) (133 66) (134 13) (146 29) (147 500)
(148 81) (182 1) (195 2) (196 1) (197 1)
(198 2) (206 20) (207 40) (209 7) (210 1)
(211 2) (212 1) (213 2) (214 2) (219 29)
(220 67) (221 37) (222 87) (223 19) (224 8)
(225 1) (228 1) (238 1) (239 8) (240 2)
(241 2) (244 2) (245 3) (246 5) (250 7)
(251 4) (254 1) (255 1) (256 1) (257 1)
(258 1) (259 2) (260 6) (268 1) (276 1)
(292 2) (293 7) (294 93) (295 28) (296 14)
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(312 1) (314 1) (318 1) (319 1) (320 1)
(322 2) (323 8) (324 4) (325 4) (326 2)
(327 2) (328 1) (329 1) (330 1) (331 1)
(332 1) (333 1) (334 2) (335 1) (336 2)
(337 2) (338 2) (339 2) (340 2) (341 2)
(342 2) (343 2) (344 2) (345 2) (346 2)
(347 2) (348 2) (349 2) (350 1) (351 1)
(352 2) (353 3) (354 1) (355 2) (356 2)
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(362 1) (363 1) (364 1) (365 1) (366 1)
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(385 1) (387 1) (398 1) (406 1) (407 1)
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(444 1) (445 1) (446 1) (448 1) (449 1)
(450 1) (451 1) (452 1) (453 2) (454 1)

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(586   1)

NAME:13C_1281.6_1313EC07_Ethanolamine (3TMS)
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer |RI:1282 |RT:1282
CASNO:128002-11-1
RI:1282
RT:6.144
SOURCE:C:\KOPKA\AMDIS32\LIB\File2.msp
NUM PEAKS:  147
( 79  93) ( 87  108) ( 94  16) (100  30) (101  24)
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(144  15) (157  11) (160   5) (161   5) (172   6)
(174  36) (175 1000) (176 177) (180  30) (183   4)
(190   1) (198   5) (202   3) (203  11) (204  29)
(212   6) (217   9) (222   2) (231   9) (233   4)
(242  15) (244  26) (245  13) (252  15) (260   6)
(262  26) (263  15) (264  19) (276   8) (277   4)
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(291  12) (296  10) (298  27) (306  24) (307   6)
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(333   6) (335  40) (336  41) (343  16) (344   5)
(346   1) (347  13) (349  17) (354  27) (355  18)
(360  19) (361  34) (362  15) (363  10) (364   9)
(368   1) (369  26) (372  13) (374  20) (376  41)
(388  14) (393  16) (398  11) (399  15) (401   3)
(402   7) (405  16) (406   6) (408   9) (409  17)
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(573   9) (577  29) (579  12) (582   4) (583  21)
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(598   3) (599  12)

NAME:13C_1283.2_1313EC11_Urea (2TMS)
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:127002-11-1
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RI:1283
RT:6.186
NUM PEAKS: 410
(70 54) (71 41) (72 86) (73 263) (74 200)
(75 57) (76 9) (77 9) (78 36) (79 62)
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(86 27) (87 54) (90 9) (92 6) (93 9)
(94 8) (95 6) (97 7) (98 4) (99 26)
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(415 6) (416 5) (417 6) (419 6) (420 4)

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(460    6) (461    5) (462    6) (463    9) (464    5)
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(477    7) (479    6) (480    5) (482    7) (484    7)
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(492    5) (493    5) (495    3) (498    8) (499    7)
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NAME:13C_2223.0_1313EC16_Tryptophan (3TMS)
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:223001-11-1
RI:2223
RT:13.883
NUM PEAKS:  161
( 72   59) ( 73  320) ( 74  110) ( 75  153) ( 76   19)
( 80   12) ( 87   41) ( 88   38) ( 89   48) ( 95   15)
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(124    8) (130    8) (136   10) (137   23) (138   38)
(139   22) (141   18) (143   10) (151    7) (153   12)
(157    7) (162   12) (167    7) (170    4) (173    7)
(174    5) (175   11) (177    8) (179   15) (195    6)
(196    7) (197    8) (200    4) (203   14) (204   11)
(209   27) (210  108) (211 1000) (212   79) (213   28)
(216    7) (217    7) (219    6) (229    5) (231    4)
(232    5) (237   11) (240    8) (247    4) (249    5)
(251    6) (258    7) (259    4) (263    5) (270    5)
(274    5) (276    3) (280    6) (281    5) (290    4)
(291    6) (292    5) (294    3) (295    4) (307    3)
(313    5) (314    7) (316    5) (317    5) (329    2)
(330    4) (334    4) (335    4) (351    5) (352    2)
(353    4) (355    7) (373    4) (378    3) (379    4)
(384    3) (386    4) (388    3) (391    3) (396    4)
(397    4) (405    3) (407    6) (408    6) (410    4)
(413    5) (417    6) (418    5) (422    9) (424    4)
(425    2) (426    6) (427    2) (431    3) (433    4)
(438    3) (441    4) (442    4) (445    3) (446    5)
(447    5) (448    3) (455    4) (462    4) (465    4)
(467    1) (471    6) (475    4) (477    5) (479    2)
(481    3) (482    5) (486    4) (488    5) (489    5)
(493    3) (496    7) (497    4) (498    3) (499    4)
(500    3) (502    3) (509    3) (513    3) (516    4)
(517    2) (518    2) (520    4) (523    4) (527    2)
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(532 4) (536 4) (537 2) (538 4) (541 4)
(542 3) (543 6) (546 3) (547 3) (550 2)
(552 4) (555 3) (558 2) (564 3) (566 3)
(567 4) (571 2) (573 2) (574 2) (591 2)
(595 2)

NAME:13C_2767.9_1313EC16_
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:277004-11-1
RI:2767
RT:16.765
NUM PEAKS: 93
(70 41) (72 34) (73 1000) (74 107) (76 39)
(78 24) (82 14) (83 31) (84 35) (91 22)
(92 19) (93 18) (97 17) (98 22) (99 25)
(100 21) (102 40) (103 55) (105 32) (106 48)
(107 56) (111 34) (112 80) (113 31) (117 32)
(118 68) (124 32) (126 12) (127 18) (129 47)
(131 35) (138 16) (139 31) (140 162) (141 348)
(142 16) (145 24) (146 55) (151 18) (152 13)
(153 15) (154 42) (155 21) (167 11) (168 21)
(169 148) (170 718) (171 19) (173 18) (174 266)
(176 24) (178 130) (179 769) (180 79) (181 67)
(183 20) (193 399) (194 30) (195 33) (196 13)
(197 33) (198 18) (206 179) (207 48) (211 32)
(212 26) (213 52) (214 15) (215 10) (216 12)
(223 15) (224 17) (241 23) (243 12) (249 26)
(254 10) (270 18) (271 20) (272 22) (273 35)
(274 12) (282 12) (283 12) (347 10) (348 12)
(385 11) (404 17) (405 10) (429 8) (436 11)
(437 18) (494 10) (523 15)

NAME:13C_1915.4_2119DC05_Lysine (4TMS)
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:192003-11-1
RI:1915
RT:28.691
NUM PEAKS: 222
(40 3) (41 58) (42 5) (43 19) (44 18)
(45 84) (46 5) (47 6) (50 2) (51 8)
(52 5) (53 14) (54 2) (55 59) (56 10)
(57 104) (58 19) (59 126) (60 15) (61 8)
(62 1) (63 4) (64 3) (65 13) (66 5)
(67 20) (68 2) (69 8) (70 3) (72 25)
(73 1000) (74 116) (75 82) (76 7) (77 23)
(78 6) (79 20) (80 3) (81 9) (82 3)
(83 6) (86 12) (87 139) (88 21) (89 85)
(90 5) (91 34) (92 4) (93 8) (94 2)
(95 10) (96 4) (97 5) (98 2) (100 20)
(101 91) (102 73) (103 58) (105 15) (106 3)
(107 11) (108 2) (109 18) (110 4) (111 6)
(112 1) (114 7) (115 55) (116 29) (117 127)
(118 23) (120 3) (121 10) (122 2) (123 8)
(124 5) (126 1) (127 3) (128 16) (129 37)
(130 64) (131 270) (132 51) (133 59) (134 8)
(135 19) (136 5) (137 8) (138 2) (139 2)
(140 1) (141 4) (142 4) (143 11) (144 11)
(145 58) (146 65) (147 126) (148 29) (149 21)
(150 7) (151 5) (152 3) (153 7) (154 8)
(155 2) (156 14) (157 8) (158 7) (159 68)

(160 59) (161 691) (162 55) (163 36) (164 5)
(165 5) (166 1) (167 1) (170 1) (171 3)
(172 11) (173 24) (175 666) (176 117) (177 85)
(178 13) (179 6) (180 1) (185 2) (186 3)
(187 8) (188 6) (189 58) (190 23) (191 16)
(192 26) (193 5) (194 3) (199 1) (200 2)
(201 7) (202 5) (203 66) (204 22) (205 98)
(206 21) (213 1) (215 2) (217 53) (218 39)
(219 18) (220 66) (221 17) (222 8) (223 1)
(228 1) (229 1) (230 3) (231 3) (232 21)
(233 66) (234 124) (235 50) (236 15) (237 2)
(238 1) (243 1) (244 1) (245 3) (246 5)
(247 4) (249 4) (250 1) (251 1) (257 1)
(260 1) (261 16) (262 5) (263 2) (264 4)
(265 2) (271 1) (276 3) (277 3) (278 8)
(279 7) (280 2) (291 1) (292 1) (299 9)
(300 2) (301 1) (305 1) (306 1) (307 2)
(308 2) (309 1) (317 3) (318 1) (319 1)
(320 1) (321 6) (322 174) (323 39) (324 21)
(325 4) (326 1) (333 1) (334 1) (335 17)
(336 7) (337 3) (396 3) (397 1) (425 4)
(426 1) (427 1) (439 1) (440 19) (441 7)
(442 4) (443 1)

NAME:13C_1920.1_2119DC05_
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:192007-11-1
RI:1920
RT:28.753
NUM PEAKS: 81
(43 35) (44 17) (45 80) (47 12) (58 64)
(71 61) (72 24) (73 1000) (74 88) (75 149)
(76 8) (84 12) (85 35) (86 15) (113 7)
(118 24) (131 28) (132 22) (133 36) (140 3)
(147 445) (148 62) (149 62) (160 17) (169 6)
(174 17) (203 35) (204 5) (206 14) (221 34)
(223 5) (229 3) (231 6) (247 3) (248 153)
(249 33) (250 18) (259 2) (263 3) (264 12)
(277 20) (278 7) (279 5) (290 2) (291 4)
(292 8) (293 303) (294 56) (295 29) (296 4)
(297 2) (305 3) (306 12) (307 13) (308 11)
(309 4) (311 4) (319 32) (320 12) (321 8)
(324 6) (338 12) (339 3) (352 12) (353 6)
(354 3) (366 4) (367 68) (368 20) (369 7)
(370 3) (378 2) (383 32) (384 8) (385 4)
(396 22) (397 5) (468 3) (486 27) (487 8)
(488 5)

NAME:13C_1858.1_2119DC05_Lysine (3TMS)
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer |RI:1858 |RI:1858
CASNO:186002-11-1
RI:1858
RT:27.441
SOURCE:C:\KOPKA\AMDIS32\LIB\File2.msp
NUM PEAKS: 119
(44 26) (45 125) (46 12) (47 13) (48 1)
(50 1) (51 1) (52 2) (58 15) (59 185)
(60 20) (61 11) (62 1) (70 3) (72 19)
(73 789) (74 139) (76 11) (78 1) (85 4)
(86 13) (87 199) (88 34) (89 233) (90 7)

(91	2)	(92	1)	(100	27)	(101	85)	(102	28)
(103	33)	(104	19)	(106	1)	(110	1)	(113	4)
(114	6)	(115	21)	(116	16)	(118	15)	(119	8)
(120	2)	(128	2)	(130	47)	(131	76)	(133	25)
(134	5)	(135	2)	(142	1)	(144	4)	(146	49)
(147	72)	(148	26)	(149	9)	(150	2)	(156	3)
(157	1)	(158	2)	(159	13)	(160	18)	(161	210)
(162	25)	(163	11)	(164	2)	(172	6)	(173	28)
(174	66)	(175	1000)	(176	170)	(177	80)	(178	9)
(179	2)	(188	3)	(189	10)	(190	12)	(192	9)
(193	2)	(200	3)	(202	1)	(203	14)	(204	5)
(205	13)	(206	176)	(207	20)	(208	8)	(217	1)
(218	2)	(219	2)	(220	9)	(230	1)	(232	1)
(233	2)	(234	4)	(235	30)	(236	8)	(237	3)
(238	1)	(245	6)	(246	2)	(247	2)	(248	3)
(249	2)	(250	1)	(261	2)	(262	1)	(263	6)
(264	47)	(265	8)	(266	4)	(278	1)	(294	1)
(295	6)	(296	1)	(297	1)	(336	1)	(353	2)
(367	1)	(368	20)	(369	5)	(370	2)		

NAME:13C_1490.2_2119DC05_
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:149003-11-1
RI:1490
RT:20.226
NUM PEAKS: 155

(42	41)	(43	38)	(44	220)	(45	159)	(46	109)
(47	38)	(51	16)	(52	19)	(56	10)	(57	23)
(59	236)	(60	49)	(61	112)	(62	15)	(64	3)
(65	3)	(66	11)	(69	8)	(70	14)	(71	8)
(72	76)	(73	1000)	(74	208)	(75	701)	(76	80)
(77	52)	(79	27)	(80	4)	(85	8)	(86	20)
(87	35)	(88	54)	(89	68)	(90	253)	(91	31)
(92	26)	(94	9)	(99	4)	(100	14)	(101	70)
(102	28)	(104	27)	(107	5)	(113	5)	(115	13)
(116	12)	(117	25)	(118	91)	(119	64)	(122	6)
(126	7)	(129	12)	(130	16)	(132	12)	(134	36)
(135	20)	(145	14)	(146	75)	(147	952)	(148	301)
(149	96)	(150	15)	(155	3)	(158	7)	(160	4)
(161	19)	(162	116)	(163	119)	(164	154)	(165	40)
(166	17)	(174	3)	(179	14)	(180	7)	(181	5)
(183	2)	(192	191)	(193	50)	(194	21)	(195	3)
(196	5)	(200	3)	(202	3)	(204	5)	(208	40)
(209	146)	(210	26)	(211	17)	(216	2)	(220	19)
(222	5)	(224	6)	(235	21)	(237	41)	(239	3)
(241	2)	(242	3)	(252	14)	(253	67)	(254	13)
(255	8)	(256	3)	(258	2)	(260	3)	(264	3)
(271	3)	(279	3)	(280	10)	(281	135)	(282	26)
(283	16)	(284	2)	(285	2)	(287	3)	(295	3)
(297	7)	(298	30)	(299	4)	(300	9)	(303	2)
(322	4)	(327	26)	(328	7)	(329	4)	(342	2)
(345	3)	(346	2)	(349	3)	(350	2)	(354	2)
(358	3)	(407	4)	(412	3)	(413	3)	(433	2)
(445	3)	(447	5)	(449	4)	(454	3)	(459	2)
(463	2)	(474	2)	(478	3)	(491	2)	(495	2)
(503	3)	(512	2)	(533	2)	(545	2)	(553	3)
(556	2)	(562	2)	(568	3)	(570	3)	(597	3)

NAME:13C_2816.0_2119DC05_
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

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CASNO:282003-11-1
RI:2816
RT:41.157
NUM PEAKS:  36
( 46   17) ( 73 1000) ( 74   77) ( 75   76) (104  215)
(132  227) (133   65) (147  285) (148   36) (160   54)
(161   50) (174  153) (178   14) (186   13) (188   11)
(192  358) (193   75) (194   44) (206  128) (208   24)
(218   14) (220  305) (221   69) (222   23) (233   22)
(236   22) (248   74) (263   13) (277   83) (308   25)
(323   33) (336   46) (367  386) (368   92) (369   49)
(370   12)

NAME:12C_1731.5_1313EC36_Ribitol (5TMS)
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:173001-10-1
RI:1731
RT:10.548
NUM PEAKS:  84
( 70    4) ( 71    5) ( 72   21) ( 73 1000) ( 74   87)
( 75   73) ( 76    3) ( 77    3) ( 81    8) ( 83    5)
( 85    4) ( 87    8) ( 88    6) ( 89   28) ( 90    3)
( 99    5) (101   28) (102    5) (103  225) (104   22)
(105   10) (111    3) (113    6) (115    6) (116   10)
(117   95) (118    9) (119    9) (129  129) (130   16)
(131   33) (132    5) (133   70) (134   10) (135    6)
(142    3) (143   10) (145    4) (147  309) (148   49)
(149   31) (150    3) (155    6) (157   24) (158    3)
(159    3) (161    3) (163    5) (170    3) (171    3)
(175    6) (177    3) (189   55) (190   12) (191   24)
(192    4) (203   14) (204   48) (205  106) (206   22)
(207   12) (217  242) (218   65) (219   25) (220    4)
(221    9) (229    7) (231    3) (243   15) (244    4)
(277   10) (278    4) (291    4) (306    4) (307   30)
(308    9) (309    4) (317    5) (318    5) (319   50)
(320   16) (321    7) (332   10) (333    4)

NAME:12C_1316.0_1313EC36_Isoleucine (2TMS)
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:132002-10-1
RI:1316
RT:6.560
NUM PEAKS:  44
( 70   19) ( 71    7) ( 72   26) ( 73  895) ( 82    4)
( 84   12) ( 85   11) ( 86   48) ( 89    4) ( 90    8)
( 96    6) ( 97    4) ( 98   12) ( 99    7) (100  126)
(102   39) (103   21) (105    3) (112    5) (113    4)
(126    3) (128   27) (129   20) (133   34) (134    8)
(145    3) (147  137) (149   16) (156    7) (158 1000)
(159  149) (160   48) (161    5) (163    5) (170   15)
(171    3) (174    3) (203    9) (217    3) (218  142)
(232   38) (233   12) (260    7) (261    2)

NAME:12C_1436.0_1313EC36_[619; 2-(3',4'-Bishydroxyphenyl)-2-oxoethylamine
(4TMS)]
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:143003-10-1
RI:1436
RT:7.989
NUM PEAKS:  26
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(73 1000) (74 109) (82 77) (85 30) (86 334)
(87 39) (89 58) (99 28) (100 186) (102 163)
(113 38) (114 26) (117 29) (126 26) (128 32)
(130 75) (154 393) (155 90) (156 130) (158 17)
(172 55) (174 538) (175 96) (176 35) (186 32)
(227 34)

NAME:12C_1459.3_1313EC36_Homoserine (3TMS)
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:146001-10-1
RI:1459
RT:8.266
NUM PEAKS: 72
(70 8) (71 13) (72 26) (73 1000) (74 95)
(75 119) (76 11) (77 5) (82 6) (83 3)
(84 15) (85 5) (86 10) (87 9) (88 4)
(98 11) (100 107) (101 22) (102 45) (103 235)
(104 23) (105 12) (112 8) (113 4) (114 14)
(115 8) (116 7) (117 15) (119 7) (127 4)
(128 397) (129 58) (130 63) (131 43) (132 25)
(133 62) (134 10) (135 5) (137 3) (143 4)
(144 6) (145 3) (146 19) (156 7) (158 9)
(160 4) (163 4) (172 6) (174 10) (175 4)
(176 4) (178 3) (186 4) (188 8) (189 4)
(191 3) (202 32) (203 8) (204 6) (214 4)
(216 11) (217 6) (218 503) (219 112) (220 42)
(221 8) (230 17) (231 4) (232 8) (292 17)
(293 6) (320 6)

NAME:12C_1495.6_1313EC36_[815; Ethyl-3(2H)-thiophenone]
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:150003-10-1
RI:1496
RT:8.698
NUM PEAKS: 56
(72 18) (73 546) (74 61) (75 165) (76 13)
(77 10) (82 5) (84 10) (86 11) (87 6)
(88 3) (96 3) (98 18) (100 67) (101 12)
(102 9) (103 16) (104 3) (105 3) (112 9)
(114 16) (115 12) (116 8) (117 41) (118 5)
(119 5) (126 5) (128 1000) (129 133) (130 82)
(131 18) (132 10) (133 23) (134 4) (144 5)
(146 3) (148 11) (149 13) (156 7) (158 13)
(172 4) (173 3) (174 5) (188 94) (189 13)
(190 4) (200 3) (202 60) (203 12) (204 5)
(216 3) (218 10) (219 3) (230 12) (290 4)
(305 3)

NAME:12C_1514.1_1313EC36_[729; N,N-Dimethyllysine methyl ester]
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:151003-10-1
RI:1514
RT:8.860
NUM PEAKS: 29
(72 40) (73 1000) (74 101) (75 258) (82 16)
(84 893) (87 12) (89 205) (98 119) (100 81)
(105 28) (114 32) (116 18) (128 67) (131 30)
(133 46) (140 41) (147 188) (148 29) (156 104)
(157 14) (158 35) (172 23) (188 844) (189 112)
(190 28) (200 16) (230 29) (274 20)

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NAME:12C_1538.2_1313EC36_[596; N-Acetylglutamic acid (2TMS)]
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:154002-10-1
RI:1538
RT:9.048
NUM PEAKS:  61
( 72    46) ( 73   454) ( 74    75) ( 75   623) ( 76    52)
( 77    33) ( 83    17) ( 84 1000) ( 86    12) ( 87    18)
( 88    13) ( 89     9) ( 90     3) ( 91     6) (101    19)
(102    10) (103    18) (104     3) (112    10) (114     7)
(115     7) (116    31) (118     4) (129    25) (130    34)
(131    24) (132     5) (133    22) (134     3) (140    40)
(141     6) (142     9) (143     3) (144    12) (145    14)
(146    19) (147    62) (148    10) (149    13) (156    57)
(157    15) (158   202) (159    30) (160    13) (173    21)
(174   400) (175    52) (176    16) (186    68) (187     8)
(201    17) (202     3) (230    35) (231     8) (232     3)
(248    14) (249     3) (258     4) (276    33) (277     7)
(278     3)

NAME:12C_1623.5_1313EC36_[882; Ornithine (3TMS)]
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:162001-10-1
RI:1624
RT:9.710
NUM PEAKS:  109
( 70   553) ( 71    37) ( 72    35) ( 73 1000) ( 74   231)
( 75   128) ( 76    13) ( 77     5) ( 80     4) ( 82     5)
( 83     4) ( 84    13) ( 85    10) ( 86    21) ( 87    12)
( 88    15) ( 89    26) ( 90     7) ( 96     7) ( 97    14)
( 98    20) ( 99     9) (100    96) (101    19) (102   115)
(103    26) (104    11) (105     3) (108     3) (110     5)
(112     6) (113     6) (114    24) (115    75) (116    19)
(117    41) (118     7) (119     5) (126     9) (127     4)
(128    65) (129    30) (130    32) (131    25) (132    29)
(133    34) (134     7) (135     3) (140     9) (141    10)
(142   661) (143   104) (144    92) (145    12) (146    22)
(147   108) (148    34) (149    14) (150     3) (152     3)
(153    16) (154    13) (155     4) (157     7) (158     7)
(159     5) (160     4) (162    60) (163    11) (164     5)
(168     3) (169    14) (170     8) (171     5) (172     9)
(173     3) (174     7) (186     4) (187     4) (188     9)
(189     5) (190     3) (191     4) (200     7) (203     3)
(204    43) (205     9) (206     4) (214     4) (215     5)
(216    33) (217    16) (218    22) (219     9) (220     3)
(227     4) (231     7) (232     8) (233     3) (241     4)
(243    31) (244    27) (245     8) (258     7) (259    12)
(260     3) (348    27) (349     9) (350     4)

NAME:12C_1640.8_1313EC36_Phenylalanine (2TMS)
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:164001-10-1
RI:1641
RT:9.844
NUM PEAKS:  63
( 71     5) ( 72    21) ( 73 1000) ( 74    94) ( 75   110)
( 76     8) ( 77    15) ( 78     5) ( 86    18) ( 87     6)
( 89    12) ( 90     6) ( 91   174) ( 92    26) ( 93     5)
(100   189) (101    26) (103    21) (104     5) (105     7)
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(115 8) (116 3) (117 15) (118 10) (119 10)
(120 12) (121 9) (130 41) (131 26) (132 31)
(133 34) (134 7) (135 9) (145 5) (146 12)
(147 159) (148 27) (149 15) (159 5) (160 18)
(161 5) (162 7) (163 10) (174 5) (176 10)
(177 12) (178 3) (190 3) (191 7) (192 282)
(193 53) (194 13) (203 7) (204 11) (205 3)
(217 4) (218 397) (219 77) (220 33) (266 24)
(267 13) (268 4) (294 6)

NAME:12C_1673.2_1313EC36_[NA]
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:167003-10-1
RI:1673
RT:10.095
NUM PEAKS: 66
(70 28) (73 1000) (74 100) (82 142) (84 9)
(98 500) (99 37) (101 8) (110 18) (114 17)
(116 11) (130 10) (140 5) (154 5) (156 50)
(157 11) (170 36) (176 4) (184 14) (186 4)
(198 5) (199 4) (200 13) (216 9) (221 5)
(230 4) (231 10) (232 9) (244 14) (249 4)
(252 4) (267 5) (279 4) (287 21) (288 458)
(289 117) (290 45) (291 8) (293 5) (318 6)
(319 6) (322 4) (324 4) (336 7) (337 4)
(344 4) (346 10) (347 6) (391 5) (398 4)
(408 5) (409 4) (410 5) (423 5) (431 5)
(439 4) (447 4) (478 4) (481 6) (490 5)
(515 5) (532 4) (548 4) (558 4) (567 3)
(570 3)

NAME:12C_1708.2_1313EC36_[499; 2-Ethyl-3-hydroxy-3-methylvaleric acid (2TMS)]
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:171003-10-1
RI:1708
RT:10.367
NUM PEAKS: 91
(70 22) (71 9) (72 25) (73 1000) (74 81)
(75 114) (79 9) (81 14) (86 12) (87 8)
(89 87) (100 46) (105 5) (112 7) (114 16)
(116 19) (117 15) (127 24) (128 52) (129 21)
(132 16) (133 28) (134 6) (135 3) (142 28)
(143 8) (144 24) (145 32) (146 9) (147 91)
(148 13) (149 6) (155 61) (158 11) (159 5)
(161 10) (171 62) (172 19) (174 22) (175 4)
(176 5) (182 5) (183 5) (185 9) (187 6)
(188 11) (202 8) (211 8) (218 16) (219 17)
(228 6) (229 9) (232 13) (242 3) (243 5)
(244 24) (245 12) (246 4) (272 31) (275 102)
(276 28) (277 12) (287 5) (288 6) (296 9)
(297 6) (298 7) (337 4) (338 4) (348 6)
(350 6) (358 3) (399 4) (411 4) (415 5)
(421 4) (422 4) (431 4) (458 6) (459 4)
(462 4) (470 3) (479 4) (483 5) (513 5)
(515 5) (543 5) (548 7) (557 5) (558 4)
(588 4)

NAME:12C_1720.9_1313EC36_[NA]
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

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CASNO:172005-10-1
RI:1721
RT:10.465
NUM PEAKS:  56
( 70   46) ( 72   90) ( 73  789) ( 74  188) ( 75 1000)
( 76   84) ( 77   54) ( 81   16) ( 83  199) ( 86   17)
( 87   41) ( 90  180) ( 94    9) (112   17) (113   31)
(115   83) (116  152) (119    8) (126   11) (131  167)
(132   24) (139   70) (140   53) (141   14) (142   24)
(145   42) (146   18) (149   13) (155  266) (156  429)
(157  135) (158  132) (159   23) (160   40) (162    9)
(171    8) (172   31) (173  617) (174   88) (175   39)
(185   10) (186   22) (187   13) (199    8) (202   14)
(223    8) (229   74) (236   10) (254    8) (255   13)
(261   10) (262    8) (268    8) (275   23) (276   13)
(285    7)

NAME:12C_1747.3_1313EC36_[612; 4-Aminobutyric acid (2TBS)]
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:175003-10-1
RI:1747
RT:10.670
NUM PEAKS:  19
( 73 1000) ( 74   93) ( 75  182) ( 78   34) ( 84  207)
(100   39) (112  314) (115   34) (129   51) (131   27)
(133   53) (147  369) (148   60) (149   43) (156   48)
(184   29) (194   48) (274  267) (275   59)

NAME:12C_1784.4_1313EC36_Glutamine (3TMS)
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:178001-10-1
RI:1785
RT:10.958
NUM PEAKS:  107
( 70   19) ( 71   11) ( 72   44) ( 73 1000) ( 74  138)
( 75  301) ( 76   23) ( 77   12) ( 81    5) ( 82    6)
( 83   35) ( 84   26) ( 85   12) ( 86   14) ( 87    8)
( 88    4) ( 89    6) ( 90    5) ( 94    3) ( 96    3)
( 97    3) ( 98   11) ( 99    7) (100   63) (101   14)
(102   11) (105    3) (110    3) (112   17) (113   11)
(114   44) (115   41) (116   37) (117   16) (118    4)
(119    5) (126   13) (127    4) (128   77) (129   23)
(130   26) (131   72) (132   26) (133   52) (134    9)
(135    5) (139   50) (140   22) (141    7) (142   22)
(143    5) (144    8) (145   36) (146   10) (147  163)
(148   32) (149   34) (150    5) (151    3) (153    3)
(154    4) (155  244) (156  775) (157  121) (158   37)
(159    5) (160    3) (167    3) (172    8) (173    9)
(174    5) (183    3) (188   15) (189    5) (190    3)
(200    3) (202    3) (203   64) (204   16) (205    6)
(211    3) (213    3) (214    3) (216    8) (218   17)
(219    5) (221    4) (227    7) (228    5) (229   27)
(230   16) (231    5) (232   10) (244    6) (245   97)
(246   22) (247    8) (257    6) (258    3) (272    5)
(273    7) (274    3) (301    7) (302    3) (347   16)
(348    5) (362    6)

NAME:12C_1843.5_1313EC36_[919; D-Xylopyranose (4TMS)]
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:184004-10-1
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RI:1844
RT:11.416
NUM PEAKS: 29
(72 19) (73 1000) (74 85) (75 114) (76 7)
(89 12) (101 32) (103 63) (117 53) (129 54)
(131 28) (133 58) (134 8) (143 20) (147 218)
(148 33) (149 27) (189 35) (191 248) (192 42)
(193 18) (203 9) (204 332) (205 69) (206 24)
(217 125) (218 28) (219 13) (305 7)

NAME:12C_1858.1_1313EC36_Lysine (3TMS)
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer |RI:1858 |RI:1858 |RI:1858
CASNO:186002-10-1
RI:1858
RT:11.530
SOURCE:C:\KOPKA\AMDIS32\LIB\File2.msp
NUM PEAKS: 99
(70 22) (71 11) (72 24) (73 1000) (74 161)
(75 194) (76 18) (77 8) (80 6) (81 3)
(82 59) (83 11) (84 200) (85 25) (86 214)
(87 28) (88 41) (89 6) (90 3) (94 14)
(95 3) (97 6) (98 12) (99 11) (100 120)
(101 22) (102 40) (103 19) (104 4) (110 7)
(111 3) (112 24) (113 10) (114 39) (115 17)
(116 20) (117 24) (118 6) (119 4) (126 7)
(127 3) (128 56) (129 15) (130 71) (131 34)
(132 21) (133 21) (134 4) (140 10) (141 3)
(142 27) (143 7) (144 15) (145 4) (146 35)
(147 67) (148 20) (149 8) (154 7) (155 5)
(156 177) (157 28) (158 20) (159 4) (160 7)
(161 3) (162 4) (166 4) (167 7) (168 39)
(169 6) (170 5) (172 19) (173 5) (174 916)
(175 169) (176 74) (177 8) (183 4) (184 8)
(186 15) (187 4) (188 4) (199 3) (200 191)
(201 35) (202 12) (216 7) (230 23) (231 6)
(232 3) (257 4) (258 46) (259 10) (260 4)
(289 6) (347 3) (362 16) (363 6)

NAME:12C_1888.7_1313EC36_[772; D-Glucose (5TMS)]
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:189005-10-1
RI:1889
RT:11.768
NUM PEAKS: 6
(169 14) (191 549) (192 88) (193 40) (204 1000)
(398 3)

NAME:12C_1892.7_1313EC36_Tyrosine (2TMS)
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:189006-10-1
RI:1893
RT:11.798
NUM PEAKS: 47
(75 399) (76 36) (77 44) (78 21) (79 15)
(80 5) (82 63) (87 36) (90 52) (91 83)
(92 10) (93 6) (95 8) (107 14) (109 5)
(118 34) (119 58) (120 7) (121 8) (123 3)
(135 43) (136 5) (137 5) (146 71) (150 8)
(151 20) (163 41) (164 19) (165 34) (166 8)
(175 12) (176 15) (177 16) (178 16) (179 1000)

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(180  231) (181   57) (208  104) (209   21) (219   75)
(220   11) (265    5) (282    3) (293    6) (310   29)
(311    7) (312    3)

NAME:12C_1973.7_1313EC36_[945; beta-D-Glucopyranose (5TMS)]
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:197002-10-1
RI:1974
RT:12.324
NUM PEAKS:  66
( 73 1000) ( 74   83) ( 75   95) ( 76    5) ( 77    5)
( 81    7) ( 83    3) ( 87    7) ( 88    4) ( 89   14)
(101   30) (102    5) (103   64) (104    5) (105    4)
(111    4) (113    3) (115    6) (116   14) (117   37)
(118    4) (119    6) (129   64) (130    8) (131   28)
(132    4) (133   56) (134    7) (135    5) (143   16)
(145    5) (147  223) (148   35) (155    4) (157    8)
(159    3) (161    3) (163    4) (169    9) (175    4)
(177    3) (189   38) (190   11) (191  266) (192   47)
(193   20) (203   12) (204  430) (205   84) (206   36)
(207    8) (217   83) (218   23) (219    9) (221    7)
(230    3) (231    9) (232    3) (233    3) (243    7)
(291    6) (305    6) (317    3) (319    3) (345    3)
(435    3)

NAME:12C_1924.5_1313EC16_Histidine (3TMS)
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:192006-10-1
RI:1925
RT:12.015
NUM PEAKS:  83
( 70   10) ( 71    5) ( 72   23) ( 73 1000) ( 74   88)
( 75   87) ( 76    5) ( 81   43) ( 82   43) ( 83   17)
( 84   18) ( 90    7) ( 96    6) ( 97    4) ( 98    8)
(104   34) (110    8) (111    6) (118    3) (119   25)
(120    3) (125    4) (126   10) (132   35) (133   21)
(134    4) (135    4) (137    3) (139    8) (147   95)
(148   15) (149    8) (150    6) (151    3) (153   47)
(154 1000) (155  214) (161   12) (165    3) (166   22)
(167    8) (180    3) (181    3) (182   14) (183    5)
(184    3) (191    9) (192    9) (193    3) (203    4)
(206   11) (207   30) (208    7) (209    3) (211    3)
(218   40) (219    8) (220   35) (222    3) (225    3)
(226   14) (227    4) (233    3) (235    4) (238   36)
(239   11) (240    4) (253    5) (254  171) (255   41)
(256   16) (257   10) (266    8) (310    4) (322    3)
(323   25) (324    7) (325    3) (328    5) (336    4)
(356   13) (357    5) (371    5)

NAME:12C_2091.2_1313EC11_myo-Inositol (6TMS)
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:209002-10-1
RI:2091
RT:13.074
NUM PEAKS:  112
( 72   16) ( 73 1000) ( 74   86) ( 75   67) ( 76    3)
( 81    9) ( 83    3) ( 85    3) ( 87    6) ( 97    3)
( 99    6) (100    3) (103   57) (108    3) (111    8)
(113    6) (115    7) (116    7) (117    8) (125    3)
(127    4) (129   76) (130   11) (131   32) (133   74)
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(134   11) (135    6) (141    4) (142    3) (143   23)
(144    6) (147  319) (148   50) (149   20) (154    3)
(155    4) (156    4) (157    7) (159    4) (167    3)
(169    4) (175   13) (177    7) (189   15) (190   13)
(191  103) (192   24) (193   10) (195    3) (201    4)
(203    7) (204   43) (205   15) (215    4) (216    5)
(217  168) (218   35) (219   17) (230    7) (231    5)
(242    3) (243    7) (244    3) (245    3) (254    3)
(260    3) (265   27) (266    9) (267    5) (291   15)
(292    6) (293    6) (304   11) (305   98) (306   32)
(307   18) (308    6) (317    8) (318   55) (319   25)
(320   11) (321    4) (331    3) (343    3) (344    3)
(345    3) (353    3) (365    3) (367    7) (368    5)
(369    3) (379    3) (391    3) (392    3) (393    5)
(394    3) (398    3) (403    3) (408    3) (417    3)
(421    3) (430    3) (431    3) (432   10) (433    8)
(434    6) (435    3) (444    3) (454    3) (506    3)
(507    5) (508    3)

NAME:12C_1293.1_1313EC75_Glycerol (3TMS)
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:129003-10-1
RI:1293
RT:6.323
NUM PEAKS:  58
( 70    4) ( 71    8) ( 72   25) ( 73 1000) ( 74   91)
( 75   90) ( 76    5) ( 85    9) ( 87   13) ( 88   13)
( 89   47) ( 90    5) ( 99    6) (101   72) (102   11)
(103  321) (104   33) (105   21) (113    7) (116   27)
(117  321) (118   34) (119   33) (120    3) (129   66)
(130   10) (131   58) (132   10) (133  231) (134   34)
(145    3) (147  583) (148   92) (149   64) (150    8)
(159    5) (161    3) (163   12) (174    4) (175   56)
(176   11) (177   33) (178    7) (189   10) (190    3)
(191   36) (192    7) (203   29) (204   43) (205  268)
(206   56) (207   29) (217   17) (218  113) (219   25)
(220   11) (221    5) (293   10)

NAME:12C_1317.6_1313EC75_Threonine (2TMS)
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:132001-10-1
RI:1318
RT:6.611
NUM PEAKS:  51
( 71   11) ( 72   29) ( 73 1000) ( 74  129) ( 75  300)
( 76   25) ( 77   17) ( 81    5) ( 85    8) ( 86    8)
( 87   49) ( 88   10) ( 89    7) ( 91    3) ( 98    9)
(100    8) (101   31) (102   18) (103   12) (104    6)
(105    5) (112    3) (114   19) (115   25) (116   18)
(117  273) (118   31) (119   15) (128    3) (129    6)
(130  206) (131   83) (132   59) (133   36) (134    8)
(135    4) (145    3) (146   73) (147  172) (148   35)
(149   15) (150    3) (176    3) (177    3) (181    4)
(203    3) (204    8) (219   76) (220   20) (221    8)
(248    8)

NAME:12C_1318.4_1313EC75_Proline (2TMS)
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:132003-10-1
RI:1318
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RT:6.620
NUM PEAKS:  32
( 70    47) ( 71    10) ( 72    46) ( 73   608) ( 80     5)
( 83     3) ( 84    13) ( 85     7) ( 86     6) ( 96     3)
( 97     3) ( 98     7) ( 99    12) (100    12) (103     9)
(113     7) (124     4) (126     4) (127     5) (128     3)
(140    12) (141     8) (142  1000) (143   137) (144    39)
(145     3) (147    80) (170    10) (175     5) (216    44)
(217     9) (244     5)

NAME:12C_1338.0_1313EC75_Succinic acid (2TMS)
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:134001-10-1
RI:1338
RT:6.850
NUM PEAKS:  32
( 72    29) ( 73   547) ( 75   415) ( 79     4) ( 86    13)
( 87     9) ( 89    10) (101     9) (102     4) (113     6)
(115    12) (116    18) (117    14) (129    95) (130     4)
(131    23) (133    46) (143     5) (145     5) (147  1000)
(148   154) (157     4) (163     3) (172    44) (173    22)
(174     4) (175    14) (218     6) (247    79) (248    16)
(249     7) (262     3)

NAME:12C_1378.1_1313EC75_Alanine (3TMS)
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:138002-10-1
RI:1378
RT:7.321
NUM PEAKS:  54
( 70    24) ( 71    10) ( 72    28) ( 73  1000) ( 74    79)
( 84     3) ( 85     7) ( 86    12) ( 87     8) ( 98     3)
( 99     5) (100   616) (101    68) (102    26) (113     8)
(114   158) (115    32) (116    26) (117    26) (118     4)
(119    11) (131    46) (132     9) (133   154) (134    21)
(135    11) (142     3) (147   220) (148    33) (149    16)
(158    14) (159     3) (160     5) (161     3) (172    24)
(173     3) (174    14) (175    11) (187     3) (188   726)
(189   138) (190    57) (191    18) (192     3) (200     3)
(202    15) (203     3) (246     4) (261     3) (262    97)
(263    29) (264    13) (290    18) (291     6)

NAME:12C_1381.0_1313EC75_Serine (3TMS)
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:138001-10-1
RI:1381
RT:7.354
NUM PEAKS:  31
( 72    31) ( 73  1000) ( 74    96) ( 86    18) ( 88    19)
(102    16) (116    71) (118     8) (119     8) (135     6)
(147   138) (148    26) (149    19) (160     5) (163     7)
(174    15) (203    11) (204   348) (205    68) (206    27)
(207     4) (216    13) (217     6) (218   178) (219    36)
(220    16) (221     5) (278    18) (279     7) (306     9)
(307     4)

NAME:12C_1410.5_1313EC75_[700; 2-methyl-1,2-propanediol (2TMS)]
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:141003-10-1
RI:1411
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RT:7.700
NUM PEAKS: 33
(73 1000) (102 98) (104 4) (115 46) (119 8)
(131 688) (132 83) (133 109) (134 13) (135 8)
(143 36) (144 7) (145 8) (147 202) (149 44)
(150 5) (161 4) (189 3) (191 14) (203 6)
(204 7) (207 4) (217 6) (220 5) (221 24)
(222 6) (223 3) (277 10) (291 7) (292 89)
(293 26) (294 12) (335 4)

NAME:12C_1419.8_1313EC75_Alanine (BP) (3TMS)
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:142001-10-1
RI:1420
RT:7.810
NUM PEAKS: 38
(70 150) (72 50) (73 1000) (74 101) (75 344)
(76 22) (86 38) (94 11) (100 148) (101 24)
(102 20) (115 12) (116 491) (117 82) (118 21)
(119 6) (131 14) (133 51) (144 43) (145 12)
(147 332) (148 50) (149 38) (160 455) (161 52)
(162 16) (175 7) (187 5) (190 128) (191 22)
(192 9) (218 9) (233 11) (234 19) (255 8)
(262 74) (263 14) (264 5)

NAME:12C_1464.2_1313EC75_[725; 2-Ketooctanoic acid (2TMS)]
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:146003-10-1
RI:1464
RT:8.330
NUM PEAKS: 82
(70 6) (71 8) (72 26) (73 674) (74 64)
(75 249) (76 17) (77 24) (79 8) (80 3)
(81 39) (82 4) (83 38) (84 7) (85 12)
(86 3) (87 8) (89 4) (93 4) (94 12)
(95 51) (96 61) (97 16) (98 7) (99 13)
(100 6) (101 5) (102 3) (103 8) (105 4)
(109 9) (110 4) (111 17) (112 5) (113 3)
(115 8) (116 3) (117 11) (119 5) (122 18)
(123 4) (124 4) (125 21) (126 10) (127 7)
(131 20) (132 4) (133 60) (134 8) (135 6)
(136 9) (140 11) (141 7) (143 4) (147 1000)
(148 161) (149 97) (150 10) (151 3) (153 7)
(155 6) (157 12) (168 10) (169 30) (170 7)
(171 4) (184 10) (185 37) (186 6) (196 3)
(197 5) (212 73) (213 22) (214 5) (215 5)
(258 3) (259 9) (286 4) (287 81) (288 19)
(289 7) (302 2)

NAME:12C_1520.6_1313EC75_Aspartic acid (3TMS)
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:152002-10-1
RI:1521
RT:8.910
NUM PEAKS: 73
(70 42) (71 9) (72 31) (73 1000) (74 107)
(75 167) (77 8) (83 4) (85 5) (86 11)
(87 6) (88 3) (89 4) (98 10) (100 253)
(101 32) (102 17) (105 3) (114 5) (115 17)
(116 11) (117 62) (118 7) (119 12) (129 5)

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(130   29) (131   23) (132   19) (133   56) (134   10)
(135    6) (142   17) (143    7) (144    9) (145    3)
(146    5) (147  167) (148   29) (149   27) (150    3)
(158    3) (160    9) (161    3) (163   17) (164    3)
(172    9) (173    3) (174   14) (175    3) (177    4)
(188   45) (189   11) (190    7) (202   46) (203    9)
(204   13) (205    4) (216   21) (217    7) (218   80)
(220    6) (221    4) (231    6) (232  382) (233   80)
(234   38) (244    4) (245    4) (246    3) (292    5)
(306   11) (307    3) (334    5)

NAME:12C_1529.0_1313EC75_Pyroglutamic acid (2TMS)
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:153002-10-1
RI:1529
RT:8.976
NUM PEAKS:  63
( 70   20) ( 71   11) ( 72   45) ( 73  883) ( 74   81)
( 75  125) ( 76    8) ( 80    4) ( 82    6) ( 83    7)
( 84   28) ( 85   18) ( 86   24) ( 87    9) ( 88    3)
( 89    3) ( 94    3) ( 96    3) ( 97    3) ( 98    7)
( 99    9) (100   17) (101    5) (102    5) (103    8)
(105    3) (110    5) (112   25) (113    8) (114   14)
(115    8) (117   10) (119    3) (122    3) (126    3)
(129    4) (131   19) (132    5) (133   35) (134    5)
(135    3) (140   28) (141   10) (142    8) (147  160)
(148   26) (149   16) (154    9) (155    6) (156 1000)
(157  130) (158   43) (174    3) (214   12) (215    3)
(228    3) (230   84) (231   19) (232    7) (258   76)
(259   17) (260    7) (273    3)

NAME:12C_1659.6_1313EC75_[910; 2-Ketogluconic acid methoxyamine (4TMS)]
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:166002-10-1
RI:1660
RT:9.991
NUM PEAKS:  40
( 72   21) ( 73 1000) ( 74   79) ( 75   73) ( 84   21)
( 87    8) ( 89   26) (101   34) (103  168) (104   14)
(115    8) (116   13) (117  120) (118   11) (119    9)
(129   42) (131   44) (133   71) (143    8) (147  258)
(148   37) (149   24) (157   11) (158    7) (172   35)
(175   10) (189   57) (190   11) (201   91) (202   16)
(203   14) (204  275) (205  107) (206   30) (217   82)
(242    5) (256   12) (288    8) (291   16) (302    6)

NAME:12C_1755.7_1313EC75_[829; Orotic acid (3TMS)]
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:176003-10-1
RI:1756
RT:10.739
NUM PEAKS:  94
( 72   85) ( 73 1000) ( 78    4) ( 79   12) ( 80    8)
( 81    8) ( 83   17) ( 86   48) ( 91    8) ( 92    4)
( 93    9) ( 94    7) ( 97   21) (100  165) (102    9)
(104    3) (105    7) (106    5) (107    4) (108    3)
(109    3) (119    8) (120    5) (123    6) (124    4)
(131   66) (132   15) (133   66) (134   10) (135    7)
(137    4) (147  214) (148   35) (149   20) (156   10)
(158   15) (160    9) (161    5) (167    9) (174   77)
```

(175 12) (176 6) (181 8) (182 3) (188 4)
(189 8) (190 10) (191 16) (192 5) (195 8)
(213 5) (214 13) (215 5) (225 7) (226 7)
(227 3) (228 3) (239 24) (240 7) (241 5)
(245 3) (252 6) (253 74) (254 502) (255 127)
(256 44) (257 5) (268 4) (269 60) (270 27)
(271 7) (272 3) (282 11) (283 5) (285 3)
(299 4) (305 8) (306 8) (313 3) (327 4)
(328 3) (329 8) (330 3) (333 7) (341 3)
(343 4) (344 4) (356 22) (357 131) (358 40)
(359 16) (371 8) (372 12) (373 4)

NAME:12C_1758.1_1313EC75_[636; 4R-Acetamido-2,3-(Z)-epoxy-4-(E)-hydroxycyclohexane (1TMS)]
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:176005-10-1
RI:1758
RT:10.757
NUM PEAKS: 89
(70 1000) (71 97) (72 22) (73 525) (74 109)
(75 231) (76 21) (77 8) (80 3) (82 5)
(83 20) (84 97) (85 186) (86 26) (87 17)
(88 6) (90 23) (91 3) (95 47) (96 15)
(97 8) (98 31) (99 122) (100 32) (101 21)
(102 10) (103 26) (104 3) (110 5) (111 5)
(112 9) (113 18) (114 14) (115 27) (116 28)
(117 20) (118 4) (122 5) (124 3) (125 30)
(126 18) (127 37) (128 10) (129 25) (130 53)
(131 27) (132 10) (139 9) (140 24) (141 54)
(143 15) (144 20) (145 7) (146 7) (147 30)
(148 6) (149 5) (151 3) (152 4) (154 8)
(155 13) (156 5) (157 19) (158 5) (159 27)
(160 4) (167 9) (168 39) (169 12) (170 10)
(171 10) (172 82) (173 16) (183 18) (184 416)
(185 65) (186 55) (187 21) (188 4) (196 5)
(211 9) (212 3) (229 4) (258 11) (259 3)
(284 3) (285 3) (286 8) (301 3)

NAME:12C_1763.9_1313EC75_Ornithine (3TMS); Arginine (BP) (3TMS)
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:176006-10-1
RI:1764
RT:10.803
NUM PEAKS: 96
(70 139) (71 16) (72 26) (73 1000) (74 173)
(75 186) (76 17) (77 7) (80 9) (82 3)
(83 5) (84 9) (85 10) (86 210) (87 38)
(88 14) (90 15) (91 3) (96 9) (97 17)
(98 15) (99 10) (100 115) (101 18) (102 36)
(103 13) (104 4) (110 5) (112 10) (113 10)
(114 20) (115 19) (116 22) (117 24) (118 5)
(119 3) (126 7) (128 43) (129 11) (130 75)
(131 48) (132 27) (133 17) (134 4) (140 7)
(141 7) (142 188) (143 30) (144 28) (145 5)
(146 60) (147 94) (148 31) (149 13) (150 3)
(152 4) (153 6) (154 23) (155 4) (156 5)
(157 3) (158 13) (159 26) (160 14) (161 12)
(162 8) (169 12) (170 13) (171 5) (172 45)
(173 9) (174 697) (175 129) (176 59) (177 7)
(186 203) (187 47) (188 15) (189 3) (200 11)

(201 3) (204 5) (213 3) (215 4) (216 33)
(217 7) (218 4) (243 9) (244 62) (245 14)
(246 5) (258 18) (259 7) (348 37) (349 12)
(350 5)

NAME:12C_1769.9_1313EC75_Glycerol-3-phosphate (4TMS)
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:177002-10-1
RI:1770
RT:10.850
NUM PEAKS: 108
(71 7) (72 27) (73 1000) (74 86) (77 15)
(85 7) (88 6) (91 5) (99 6) (101 102)
(103 118) (104 12) (105 12) (107 5) (113 20)
(115 23) (116 25) (117 24) (119 13) (121 7)
(123 3) (129 69) (131 56) (132 8) (133 113)
(134 15) (135 33) (136 4) (137 13) (139 3)
(147 155) (148 23) (149 21) (150 3) (151 9)
(153 3) (163 8) (165 4) (177 3) (179 4)
(181 17) (182 3) (183 8) (191 16) (193 20)
(194 4) (195 18) (196 3) (197 6) (203 11)
(205 8) (207 32) (208 7) (209 6) (210 3)
(211 93) (212 17) (213 11) (220 3) (225 20)
(226 6) (227 18) (228 3) (241 17) (242 4)
(243 10) (253 6) (255 4) (256 19) (269 6)
(283 6) (284 3) (285 19) (286 5) (287 3)
(298 18) (299 175) (300 47) (301 25) (302 5)
(313 4) (314 11) (315 42) (316 12) (317 6)
(327 4) (328 9) (341 14) (342 7) (343 3)
(356 18) (357 112) (358 34) (359 16) (360 3)
(369 3) (370 21) (371 7) (372 4) (373 9)
(374 3) (386 3) (387 12) (388 5) (389 5)
(444 4) (445 17) (446 7)

NAME:12C_1802.0_1313EC75_[706; Xylitol (5TMS)]
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:180002-10-1
RI:1802
RT:11.098
NUM PEAKS: 69
(72 14) (73 1000) (74 101) (75 140) (87 4)
(88 4) (89 11) (100 4) (101 12) (102 11)
(103 34) (104 6) (113 5) (115 6) (116 8)
(117 40) (118 6) (119 5) (128 13) (129 50)
(130 10) (131 19) (132 5) (133 35) (134 5)
(135 4) (141 21) (142 6) (143 19) (144 10)
(145 3) (147 141) (148 21) (149 19) (155 5)
(157 23) (169 9) (189 20) (190 4) (191 33)
(192 5) (203 3) (205 16) (206 3) (215 9)
(217 54) (218 13) (219 11) (220 3) (221 7)
(229 8) (230 6) (231 7) (232 4) (243 3)
(245 3) (246 4) (257 39) (258 10) (259 4)
(272 4) (303 6) (319 6) (347 5) (362 3)
(436 5) (437 23) (438 11) (439 5)

NAME:12C_1813.0_1313EC75_Glyceric acid-3-phosphate (4TMS)
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:181003-10-1
RI:1813
RT:11.184

```
NUM PEAKS:  69
( 72   28) ( 73 1000) ( 74   80) ( 75  112) ( 77   20)
( 87    9) ( 89   17) ( 90    5) (101   87) (102   11)
(104    7) (105   13) (107    6) (115   16) (116   29)
(117   17) (121   10) (132    8) (133  101) (134   16)
(135   32) (137   15) (141    4) (144    6) (147  252)
(148   39) (149   26) (151   11) (153    5) (181   19)
(189   15) (190    5) (193   19) (194    5) (195   18)
(207   28) (211  118) (212   20) (213   12) (214    5)
(225   19) (226    7) (227   99) (228   17) (229    9)
(243    5) (298   12) (299  125) (300   36) (301   17)
(302    3) (315   45) (316   14) (317    8) (341   11)
(342    6) (343    6) (352    3) (356   14) (357   66)
(358   20) (359    8) (386   10) (387   32) (388   14)
(389    8) (458    6) (459   13) (460    6)

NAME:12C_1819.8_1313EC75_Ornithine (4TMS)
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:182002-10-1
RI:1820
RT:11.237
NUM PEAKS:  105
( 70   24) ( 71    9) ( 72   19) ( 73 1000) ( 74  117)
( 80    3) ( 82    3) ( 83    4) ( 84   12) ( 85   10)
( 86  112) ( 87   16) ( 88    7) ( 90    5) ( 91    3)
( 96    5) ( 98   14) (100  104) (101   18) (102   46)
(103   19) (104    4) (110    9) (112   17) (113    9)
(114   31) (115   23) (116   16) (117   19) (118    5)
(119    6) (124    3) (126   19) (127   13) (128   53)
(130   59) (131   31) (132   29) (133   26) (134    6)
(140   12) (141   12) (142  898) (143  127) (144   49)
(145    6) (146   41) (152    7) (153    4) (154    6)
(156    4) (158    9) (159    6) (160   12) (161    5)
(162    4) (168    4) (169   10) (170    6) (172   38)
(173    9) (174  294) (175   54) (176   29) (177    4)
(186   13) (187   12) (188    9) (189   15) (190    5)
(191    7) (198    3) (200   57) (201   14) (202   10)
(203    8) (204   19) (205    5) (214   30) (215   10)
(216   33) (217   12) (218   17) (219    4) (220    5)
(226    3) (230    4) (232    4) (241    6) (242    4)
(243    3) (244    6) (258   21) (259   21) (260    6)
(303    4) (315    5) (316    3) (330    7) (331    3)
(405    3) (419    3) (420   15) (421    7) (422    4)

NAME:12C_1827.9_1313EC75_Arginine (5TMS)
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:183001-10-1
RI:1828
RT:11.300
NUM PEAKS:  43
( 70  162) ( 71   26) ( 73 1000) ( 74   25) ( 84   87)
( 85   30) ( 98   17) (100   88) (112    7) (114   17)
(115   41) (125    7) (126    5) (127   21) (128   15)
(130   10) (132   15) (140   41) (141  122) (142  239)
(143   17) (155   25) (156   26) (157  667) (158   83)
(167    9) (168   14) (171   25) (172   33) (173    5)
(187   13) (188    7) (215    7) (216   13) (240   10)
(244   15) (256  223) (257   50) (258   15) (292    3)
(358    4) (371    2) (373    5)
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NAME:12C_1835.3_1313EC75_[731; Erythrose (3TMS)]
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:184003-10-1
RI:1835
RT:11.358
NUM PEAKS: 137

(70	8)	(71	7)	(72	22)	(73	1000)	(74	89)
(75	143)	(76	9)	(77	11)	(80	4)	(81	3)
(82	6)	(83	37)	(84	87)	(85	15)	(86	5)
(87	12)	(88	6)	(89	43)	(90	4)	(91	3)
(94	3)	(96	12)	(97	4)	(98	4)	(99	15)
(100	21)	(101	33)	(102	9)	(103	93)	(104	10)
(108	6)	(109	3)	(110	3)	(111	10)	(112	4)
(113	26)	(114	11)	(115	25)	(116	32)	(117	131)
(118	14)	(119	14)	(122	3)	(124	3)	(126	3)
(127	5)	(128	20)	(129	84)	(130	18)	(131	42)
(132	10)	(133	74)	(134	11)	(135	10)	(136	6)
(141	4)	(142	7)	(143	22)	(144	13)	(145	7)
(146	3)	(147	250)	(148	40)	(149	47)	(150	10)
(151	3)	(152	3)	(155	4)	(156	45)	(157	22)
(158	12)	(159	27)	(163	20)	(164	4)	(168	12)
(173	29)	(174	8)	(175	7)	(177	10)	(182	11)
(183	4)	(184	12)	(185	4)	(186	4)	(189	45)
(190	11)	(191	75)	(192	13)	(193	6)	(196	7)
(197	5)	(198	23)	(199	4)	(200	3)	(201	5)
(202	17)	(203	42)	(204	68)	(205	21)	(206	7)
(207	3)	(210	9)	(211	6)	(215	8)	(216	4)
(217	103)	(218	89)	(219	23)	(220	7)	(221	3)
(224	7)	(226	54)	(227	9)	(228	3)	(229	3)
(230	10)	(231	43)	(232	11)	(233	24)	(234	5)
(239	6)	(240	3)	(245	3)	(246	8)	(258	4)
(272	5)	(300	10)	(301	3)	(314	5)	(316	7)
(317	3)	(318	10)	(319	6)	(320	3)	(329	24)
(330	7)	(404	5)						

NAME:12C_1869.1_1313EC75_Fructose methoxyamine (5TMS)
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:187002-10-1
RI:1869
RT:11.621
NUM PEAKS: 87

(70	5)	(71	5)	(72	19)	(73	1000)	(74	83)
(75	63)	(76	3)	(82	4)	(84	16)	(85	5)
(87	7)	(88	6)	(89	47)	(90	4)	(99	4)
(100	10)	(101	17)	(102	5)	(103	351)	(104	35)
(105	17)	(113	4)	(114	8)	(115	7)	(116	5)
(117	54)	(118	6)	(119	8)	(126	3)	(128	3)
(129	40)	(130	8)	(131	22)	(132	4)	(133	71)
(134	9)	(135	5)	(142	5)	(143	8)	(145	5)
(147	183)	(148	30)	(149	19)	(157	7)	(158	3)
(159	3)	(163	8)	(172	14)	(173	17)	(174	4)
(175	6)	(177	4)	(189	30)	(190	7)	(191	16)
(192	3)	(201	8)	(202	6)	(203	4)	(204	14)
(205	22)	(206	5)	(207	5)	(214	3)	(216	5)
(217	222)	(218	46)	(219	22)	(220	3)	(221	6)
(231	6)	(244	3)	(256	3)	(260	3)	(262	4)
(263	6)	(277	17)	(278	6)	(279	3)	(291	4)
(306	3)	(307	76)	(308	23)	(309	11)	(335	5)
(364	11)	(365	4)						

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NAME:12C_1879.6_1313EC75_Fructose methoxyamine (BP) (5TMS)
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:188004-10-1
RI:1880
RT:11.703
NUM PEAKS:  81
( 70    6) ( 71    5) ( 72   19) ( 73 1000) ( 74   88)
( 75   78) ( 82    7) ( 84   35) ( 85    7) ( 86    4)
( 87    8) ( 88    6) ( 89   72) ( 90    6) ( 99    4)
(100   12) (101   21) (102    5) (103  365) (104   38)
(105   26) (113    6) (114   26) (115    9) (116    8)
(117   55) (118    7) (119   11) (126    3) (128    4)
(129   40) (133   59) (134    8) (135    5) (142    7)
(143    9) (145    6) (147  216) (148   35) (156    3)
(159    3) (172    9) (173   17) (175    7) (177    3)
(188    3) (189   29) (190    7) (191   18) (192    3)
(198    3) (201    7) (202    8) (203    5) (204   16)
(205   28) (206    6) (207    5) (216    5) (217  255)
(218   55) (219   25) (221    7) (231    6) (244    6)
(245    3) (262   14) (263    9) (264    3) (277   18)
(278    6) (279    3) (291    3) (306    4) (307   86)
(308   26) (309   12) (335    5) (336    3) (364   12)
(365    4)

NAME:12C_1931.9_1313EC75_Sorbitol (6TMS); Glucitol (6TMS)
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:193001-10-1
RI:1932
RT:12.063
NUM PEAKS:  90
( 70    3) ( 71    4) ( 72   19) ( 73 1000) ( 74   88)
( 75   66) ( 76    3) ( 81    3) ( 83   10) ( 85    4)
( 87    8) ( 88    5) ( 89   26) ( 90    3) ( 97    6)
( 99    4) (101   24) (102    5) (103  175) (104   17)
(105    9) (111    3) (113    5) (115    7) (116    7)
(117  100) (118   10) (119    8) (127    3) (129   83)
(130   10) (131   27) (132    4) (133   59) (134    8)
(135    6) (141    3) (143   14) (145    4) (147  316)
(148   51) (149   33) (150    4) (155    4) (157   60)
(158    8) (159    5) (163    5) (169    4) (175    9)
(177    5) (183    7) (189   34) (190    9) (191   32)
(192    6) (193    3) (203    5) (204   41) (205  148)
(206   30) (207   15) (217  153) (218   32) (219   14)
(220    3) (221    9) (229   15) (230    6) (231   16)
(232    4) (255    6) (259    4) (277    7) (278    4)
(291    7) (305    8) (306    5) (307   24) (308    7)
(309    3) (318    7) (319  118) (320   38) (321   17)
(322    4) (331    8) (332    3) (345    5) (421    3)

NAME:12C_1956.6_1313EC75_[793; D-Galactono-1,4-lactone (4TMS)]
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:196004-10-1
RI:1957
RT:12.219
NUM PEAKS:  124
( 70   11) ( 71    5) ( 72   20) ( 73 1000) ( 74   85)
( 75  117) ( 76   10) ( 77    8) ( 81   12) ( 82   17)
( 83    5) ( 85    6) ( 86    4) ( 87    7) ( 88    5)
( 89   50) ( 90    5) ( 91    6) ( 96    3) ( 97    4)
( 98    3) ( 99    7) (100   11) (101   24) (102   11)
```

(103 101) (104 11) (105 14) (109 5) (110 5)
(111 7) (112 3) (113 5) (114 5) (115 11)
(116 11) (117 54) (118 7) (119 10) (126 4)
(127 5) (128 5) (129 88) (130 30) (131 31)
(132 7) (133 56) (134 8) (135 6) (139 3)
(141 3) (142 12) (143 18) (144 5) (145 8)
(146 4) (147 165) (148 48) (149 26) (150 4)
(153 4) (154 3) (155 12) (156 4) (157 29)
(158 12) (159 5) (160 15) (161 14) (162 3)
(163 10) (168 4) (169 55) (170 34) (171 9)
(172 4) (173 4) (174 8) (177 3) (183 4)
(186 9) (189 34) (190 8) (191 21) (192 4)
(200 3) (201 3) (203 7) (204 48) (205 21)
(206 6) (207 3) (215 4) (216 5) (217 218)
(218 47) (219 31) (220 5) (221 4) (228 3)
(229 7) (230 4) (231 6) (232 3) (242 6)
(243 28) (244 13) (245 8) (246 4) (247 4)
(248 3) (259 3) (260 4) (271 18) (272 5)
(273 3) (291 3) (331 5) (332 13) (333 5)
(360 4) (361 43) (362 15) (363 7)

NAME:12C_1999.3_1313EC75_Gluconic acid (6TMS)
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:200001-10-1
RI:1999
RT:12.490
NUM PEAKS: 87
(72 18) (73 1000) (74 88) (75 67) (76 3)
(81 7) (82 8) (83 28) (84 8) (85 10)
(89 14) (96 5) (97 26) (98 5) (101 15)
(102 14) (103 98) (104 9) (105 6) (111 12)
(113 4) (115 4) (117 56) (118 6) (119 7)
(125 6) (129 48) (130 12) (131 27) (132 4)
(133 53) (134 7) (135 6) (143 30) (144 3)
(145 3) (147 310) (148 49) (149 31) (150 3)
(153 3) (157 19) (161 3) (169 5) (171 6)
(175 5) (189 32) (190 9) (191 18) (204 32)
(205 58) (206 12) (207 10) (217 66) (218 14)
(219 12) (220 4) (221 14) (222 3) (229 7)
(230 3) (231 4) (245 5) (277 10) (278 3)
(291 8) (292 59) (293 18) (294 8) (305 25)
(306 9) (307 8) (318 3) (319 27) (320 9)
(331 4) (332 7) (333 55) (334 18) (335 8)
(345 3) (359 8) (360 3) (423 6) (433 3)
(434 3) (435 4)

NAME:12C_2048.2_1313EC75_Hexadecanoic acid (1TMS)
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:205001-10-1
RI:2048
RT:12.799
NUM PEAKS: 111
(70 27) (71 43) (72 51) (73 944) (74 111)
(75 1000) (76 74) (77 54) (79 26) (80 4)
(81 70) (82 10) (83 74) (84 29) (85 30)
(86 14) (87 11) (88 8) (89 29) (90 5)
(91 11) (93 23) (94 4) (95 65) (96 10)
(97 54) (98 41) (99 27) (100 5) (101 17)
(102 6) (105 29) (106 3) (107 12) (109 19)
(110 4) (111 25) (112 12) (113 6) (115 10)

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(116   67) (117  969) (118   95) (119   41) (121    9)
(123    6) (125    7) (126    5) (127    5) (128    4)
(129  492) (130   64) (131  174) (132  459) (133   90)
(134   22) (135    9) (137    3) (139    5) (140    5)
(141    4) (142    4) (143   45) (144    7) (145  233)
(146   31) (153    5) (154    7) (155    6) (157   15)
(158    4) (159   26) (167    3) (168    3) (171   24)
(172    4) (173    8) (174    6) (185   33) (186    5)
(187   21) (188    6) (195    4) (199   10) (201   53)
(202   10) (203    3) (213   10) (214    3) (215    8)
(216    3) (227   11) (228    3) (229   12) (230    3)
(241    5) (243   12) (244    3) (257    7) (269   15)
(270    4) (271    4) (283    3) (285   15) (286    4)
(312   15) (313  233) (314   66) (315   17) (328   26)
(329    8)

NAME:12C_2087.4_1313EC75_[756; beta-D-Methylglucopyranoside (4TMS)]
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:209004-10-1
RI:2087
RT:13.047
NUM PEAKS:  68
( 70    6) ( 72   21) ( 73 1000) ( 74   88) ( 75   70)
( 81    6) ( 82    6) ( 83    7) ( 86    6) ( 88    3)
( 89   78) ( 90    7) ( 97    4) (100   42) (101   34)
(102   16) (103   61) (105   11) (115    8) (116   15)
(117   36) (118    4) (129   57) (130   10) (131   27)
(132   12) (133   44) (134    7) (135    6) (142    5)
(143   13) (145    7) (147  212) (148   60) (149   28)
(155    5) (157   30) (160    9) (161    5) (163    8)
(169    8) (172   10) (187    3) (189   31) (190    9)
(201    5) (203   12) (204  342) (205   83) (206   32)
(207    8) (216    3) (217   56) (218   16) (219    8)
(220   69) (221   18) (222    6) (229    6) (230    5)
(231    8) (233   10) (243    8) (244    5) (247    3)
(319   64) (320   23) (321   11)

NAME:12C_2064.0_1191EC10_[770; 3,4,6-Trishydroxyphenylethanolamine (5TMS)]
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:206001-10-1
RI:2064
RT:13.339
NUM PEAKS:  191
( 70   28) ( 71   17) ( 72   20) ( 75  211) ( 77   38)
( 81   37) ( 82   17) ( 83   13) ( 86  301) ( 87   27)
( 88    5) ( 90    3) ( 91   11) ( 93   24) ( 95   10)
( 96    4) ( 98    7) (100  150) (101   32) (102   84)
(105    5) (106    4) (107    6) (109   20) (112    6)
(113    9) (114   12) (115   15) (116   15) (117  181)
(118   16) (119   11) (121    7) (122    4) (123   14)
(124    3) (125    9) (128    8) (130   62) (131   20)
(132   25) (133   44) (134    5) (135    6) (136    7)
(137    4) (139    4) (142   13) (143   10) (144   13)
(146   19) (147   61) (148   15) (149   16) (150    4)
(151    4) (156    5) (157    7) (158   34) (161    3)
(162    6) (164    5) (170    6) (171   12) (172   37)
(173    5) (174 1000) (175  168) (176  129) (177   15)
(182    6) (186    8) (187   14) (188   10) (189    6)
(191   11) (196    5) (199    6) (200    9) (201    5)
(202    8) (203    4) (204   16) (207    9) (208    7)
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(211    8) (213    5) (217    8) (220    8) (226    4)
(227   13) (233    7) (234    3) (235    3) (243    6)
(244    4) (246    3) (248    8) (250    3) (252    9)
(257   13) (258    8) (259    9) (261    6) (262    3)
(264    8) (266   11) (269    6) (270    3) (271    3)
(275    8) (276    6) (284    5) (285    7) (290    3)
(291    3) (301    3) (303    5) (307    3) (309    4)
(310    4) (311    3) (313    5) (317    5) (321    7)
(322    5) (333    8) (334    4) (335    5) (337    3)
(338    6) (339    3) (343    3) (344    4) (345    3)
(346    3) (347    4) (348   10) (353    3) (354    3)
(359    8) (361    8) (365    4) (367    3) (376    3)
(377    5) (378    4) (389    4) (390    6) (392    5)
(395    5) (411    4) (420    6) (421    4) (424    5)
(425    3) (428    3) (435    3) (448   13) (449   47)
(450   26) (451   18) (466    6) (467    3) (469    4)
(470    5) (473    3) (475    4) (478    4) (484    3)
(488    5) (493    3) (495    5) (498    7) (500    5)
(507    3) (512    4) (514    5) (515    6) (525    3)
(529    5) (530    3) (533    6) (534    8) (543    6)
(547    5) (553    4) (557    4) (567    3) (575    3)
(595    4)
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NAME:12C_2023.2_1160EC43_[766; beta-D-Methylglucopyranoside (4TMS)]
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:203003-10-1
RI:2023
RT:13.133
NUM PEAKS:  92
( 70    4) ( 71    3) ( 72   17) ( 73 1000) ( 74   84)
( 75   90) ( 76    5) ( 77    5) ( 81    5) ( 83    4)
( 84    7) ( 85    4) ( 86    3) ( 87    4) ( 88    3)
( 89   75) ( 90    7) ( 91    7) ( 97    4) ( 99    5)
(100   46) (101   23) (102   17) (103   75) (104    8)
(105   10) (111    3) (113    6) (115    9) (116   12)
(117   34) (118    4) (119    7) (127    3) (128    4)
(129   68) (130   13) (131   26) (132   12) (133   48)
(134    6) (135    4) (142    5) (143   15) (144    3)
(145    6) (147  176) (148   57) (149   25) (150    3)
(155    4) (157   32) (158    6) (159    4) (160    7)
(161    5) (163    7) (169    9) (170    3) (172    8)
(173    3) (174    3) (175    3) (177    3) (189   36)
(190   10) (191   22) (192    4) (203    8) (204  398)
(205   97) (206   38) (207    8) (217   85) (218   23)
(219   10) (220   80) (221   18) (222    7) (229    5)
(230    5) (231    6) (233   13) (234    3) (243    9)
(244    4) (259    6) (291    3) (305    4) (319   69)
(320   23) (321   11)
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NAME:12C_2002.2_1178EC16_[775; Dopamine (4TMS)]
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:200002-10-1
RI:2002
RT:12.973
NUM PEAKS:  186
( 70   70) ( 72   16) ( 73  932) ( 74  101) ( 75  182)
( 76   10) ( 77    8) ( 80   10) ( 82   14) ( 84   13)
( 86  211) ( 87   27) ( 88    6) ( 89    6) ( 90    4)
( 94   28) ( 95    3) ( 96   11) ( 98   21) ( 99    5)
(100  103) (101   17) (102   32) (103   14) (104    5)
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(105    5) (106    4) (110    4) (111    7) (112   23)
(113    6) (114   19) (115   15) (116   42) (117   19)
(118    7) (119    5) (121    5) (122    3) (123    3)
(126    5) (128   29) (129    9) (130   74) (131   41)
(132   16) (133   30) (134    7) (135    7) (138    3)
(139    9) (140    7) (141    3) (142  107) (143   21)
(144   17) (146   31) (147   77) (148   16) (149   20)
(150    7) (151    4) (152    9) (153    3) (154    8)
(156   11) (158   13) (159    5) (160    4) (161    5)
(163    4) (166    4) (168    9) (169    4) (170   24)
(171   14) (172   28) (173   18) (174 1000) (175  174)
(176   77) (177    9) (184   12) (186   44) (187    7)
(188    5) (190    4) (195    4) (196    4) (199    3)
(200   19) (201    6) (202    5) (203    3) (204    3)
(206    3) (208    3) (209    3) (211   10) (212    3)
(213    4) (214   45) (215   10) (216   12) (220    3)
(221    3) (222    4) (227    6) (228   14) (229    7)
(230    8) (231    3) (232    3) (244    7) (246    3)
(252    3) (258    6) (260    3) (261   20) (262    6)
(263    3) (270    3) (272    3) (274    3) (281    3)
(285    6) (286    7) (287    4) (289    8) (298    3)
(301    5) (303    3) (314    3) (317   34) (318   13)
(319    4) (320    3) (323    3) (331    3) (332    3)
(344    3) (352    3) (353    3) (357    4) (362    3)
(375   23) (376    9) (377    7) (378    3) (388    3)
(389    5) (390    6) (395    3) (397    3) (403    4)
(404    3) (408    3) (413    3) (415    3) (425    3)
(429    3) (432    3) (433    3) (436    3) (440    3)
(444    3) (455    3) (461    3) (466    3) (467    4)
(480    4) (481    4) (491    3) (502    4) (503    3)
(514    5) (517    3) (522    4) (523    3) (526    3)
(528    3) (535    3) (547    3) (549    4) (550    3)
(551    4)
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NAME:12C_1882.5_1274EC11_Mannose methoxyamine (5TMS)
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:188002-10-1
RI:1883
RT:12.225
NUM PEAKS:  114
( 72    6) ( 73 1000) ( 74   78) ( 75  158) ( 76   43)
( 77   12) ( 81    6) ( 85    3) ( 87    3) ( 88    5)
( 89   36) ( 90    3) ( 91    9) ( 93   19) ( 94    4)
( 97    5) ( 99   10) (100   10) (101   28) (102   11)
(103  139) (104   47) (105   32) (106    7) (111    3)
(113    5) (115   11) (116   17) (117  114) (118   13)
(119   16) (120    3) (121   16) (122    7) (123    6)
(126    6) (127    5) (129  183) (130   32) (131   43)
(132   15) (134    3) (135    8) (138    5) (141    3)
(142    8) (143   24) (144    5) (145   10) (147  118)
(148   19) (151    7) (154    4) (155    4) (156    3)
(157  138) (158   23) (159   11) (163   26) (164    4)
(167   20) (168    4) (169   13) (170    4) (171    7)
(173   42) (174   26) (175    7) (177    5) (182    3)
(186    9) (187    4) (189   87) (190   18) (196    3)
(197    3) (201    4) (203    8) (205  126) (206   21)
(207   11) (214    5) (215    6) (217  100) (218   18)
(219   23) (220   48) (221   14) (222    6) (223   28)
(224    4) (229   24) (230    9) (231    7) (243   16)
(244   12) (245    8) (246    4) (247   20) (248    6)
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(249    3) (257    3) (259    5) (271    4) (277    3)
(302    4) (304    5) (305    4) (306    3) (319   53)
(320   14) (321    6) (333    8) (334    3)

NAME:12C_1882.4_1160EC15_Adenine (2TMS)
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:188005-10-1
RI:1882
RT:12.217
NUM PEAKS:  37
( 73  675) ( 79   56) ( 81   27) ( 84  169) ( 86   45)
( 91  126) ( 95   59) ( 99   74) (103   15) (109  161)
(110   61) (115   31) (117   21) (119   79) (120   56)
(122   30) (137   34) (164   22) (165   80) (167   56)
(176   17) (192  219) (193   42) (227  138) (264 1000)
(265  190) (266   43) (270    9) (278  128) (279  206)
(359    9) (413   24) (431   24) (462   10) (484   19)
(500   12) (582   25)

NAME:12C_1850.9_1274EC11_[912; Tetradecanoic acid (1TMS)]
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:185004-10-1
RI:1851
RT:11.982
NUM PEAKS:  82
( 70   17) ( 71   20) ( 72   43) ( 73  681) ( 74   70)
( 75  933) ( 76   67) ( 77   47) ( 79   19) ( 81   57)
( 83   42) ( 85   16) ( 87    5) ( 89   21) ( 90    4)
( 91    7) ( 93   15) ( 95   52) ( 96    7) ( 97   34)
( 98   31) ( 99   19) (101   11) (105   29) (107    8)
(109   16) (111   17) (112    8) (115    6) (116   62)
(117 1000) (118   99) (119   40) (121    6) (123    4)
(125    5) (129  412) (130   43) (131  178) (132  449)
(133   86) (134   22) (135    5) (141    3) (143   37)
(144    3) (145  203) (146   24) (147    8) (153    3)
(154    7) (155    3) (159   26) (167    5) (171   18)
(173    8) (185   23) (186    3) (187   16) (188    4)
(199    7) (201   49) (202    8) (203    3) (204    3)
(213    9) (215   10) (216    3) (227    6) (229    3)
(241   16) (242    4) (243    7) (257   19) (284    3)
(285  222) (286   55) (287   15) (299    9) (300   30)
(301    8) (302    3)

NAME:12C_1822.5_1313EC75_Citric acid (4TMS)
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:182004-10-1
RI:1823
RT:11.258
NUM PEAKS:  87
( 70    7) ( 71    5) ( 72   35) ( 73 1000) ( 74   85)
( 75  185) ( 76   12) ( 77   22) ( 79    3) ( 83    3)
( 85    3) ( 87    4) ( 88    3) ( 95    5) ( 97    7)
( 99   17) (101    6) (111    9) (115   18) (116    9)
(117   15) (118    3) (119    5) (129   25) (130    3)
(131   28) (132    4) (133   46) (134    7) (135    6)
(139    5) (141    8) (142    3) (143   17) (145    3)
(147  288) (148   46) (149   48) (150    6) (151    4)
(157    6) (163    5) (169    5) (171    6) (183   39)
(184    6) (185   11) (189    4) (190    4) (191    5)
(201    3) (207    7) (211   46) (212    7) (213    8)
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(215 7) (217 10) (221 20) (222 5) (223 3)
(229 5) (231 11) (232 3) (245 3) (257 23)
(258 6) (259 5) (273 171) (274 39) (275 17)
(285 6) (301 4) (303 5) (305 10) (306 3)
(347 32) (348 11) (349 6) (363 22) (364 7)
(365 3) (375 26) (376 9) (377 5) (465 9)
(466 5) (467 3)

NAME:12C_1824.3_1191EC08_[570; Hypoxanthine (2TMS)]
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:182006-10-1
RI:1824
RT:11.718
NUM PEAKS: 163
(71 177) (74 499) (79 33) (80 60) (81 31)
(85 268) (86 997) (90 10) (91 279) (98 29)
(99 87) (100 809) (102 373) (104 78) (105 781)
(106 124) (107 7) (108 8) (109 35) (110 55)
(111 29) (112 89) (113 12) (114 40) (118 70)
(119 103) (120 56) (121 30) (123 111) (124 55)
(125 151) (126 50) (138 29) (140 57) (144 25)
(145 61) (152 36) (154 61) (159 15) (165 9)
(166 101) (170 15) (172 118) (173 82) (178 19)
(179 15) (180 23) (181 81) (182 30) (184 19)
(187 16) (188 70) (190 16) (191 58) (192 55)
(193 99) (194 22) (195 10) (197 22) (198 25)
(199 33) (201 48) (202 16) (203 19) (204 24)
(205 31) (206 153) (207 8) (208 22) (214 33)
(215 18) (219 19) (220 25) (226 21) (227 6)
(229 99) (230 32) (234 21) (238 30) (239 24)
(241 308) (242 128) (243 31) (244 21) (248 9)
(249 26) (250 17) (251 10) (252 20) (253 4)
(254 6) (258 222) (259 82) (260 14) (261 8)
(262 11) (263 10) (264 20) (265 1000) (266 253)
(267 101) (270 31) (277 9) (279 32) (280 326)
(281 86) (282 17) (288 12) (289 10) (303 5)
(304 10) (315 8) (316 16) (317 4) (326 4)
(329 22) (330 19) (331 25) (332 25) (337 5)
(341 10) (343 11) (351 15) (356 3) (357 9)
(378 4) (388 3) (403 7) (405 12) (406 19)
(407 7) (421 10) (422 18) (423 26) (424 3)
(431 6) (435 4) (439 4) (445 8) (446 6)
(450 6) (451 4) (458 8) (462 11) (469 7)
(471 3) (476 4) (501 7) (524 5) (529 4)
(530 6) (537 4) (538 6) (543 4) (561 6)
(564 3) (568 8) (569 7) (571 6) (575 4)
(581 4) (582 3) (595 3)

NAME:12C_1771.1_1274EC11_[812; D-Xylofuranose (4TMS)]
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:177004-10-1
RI:1771
RT:11.367
NUM PEAKS: 78
(70 6) (72 13) (73 1000) (74 81) (75 94)
(76 4) (77 5) (79 3) (81 10) (83 6)
(84 6) (85 3) (87 4) (89 5) (95 4)
(97 4) (99 7) (103 12) (109 4) (111 5)
(113 5) (115 4) (116 4) (117 30) (118 3)
(119 6) (127 4) (128 3) (129 28) (130 3)

(131 11) (133 47) (141 4) (142 7) (143 19)
(144 7) (145 6) (147 226) (148 35) (149 35)
(150 4) (155 5) (157 7) (159 6) (161 3)
(163 9) (169 20) (170 4) (171 3) (177 4)
(189 5) (191 38) (203 15) (204 5) (205 3)
(215 3) (217 523) (218 137) (219 55) (220 9)
(221 5) (231 5) (232 56) (233 15) (234 6)
(243 6) (245 6) (255 3) (257 16) (258 4)
(271 4) (305 16) (306 5) (307 3) (318 3)
(450 18) (451 10) (452 5)

NAME:12C_1710.6_1274EC17_[817; Ribitol (5TMS)]
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer |RI:1711 |RI:1711
CASNO:171008-10-1
RI:1711
RT:10.896
SOURCE:C:\KOPKA\AMDIS32\LIB\File2.msp
NUM PEAKS: 148
(72 16) (73 1000) (74 86) (75 260) (76 15)
(77 32) (81 6) (83 29) (88 7) (89 11)
(95 16) (97 26) (101 105) (102 14) (103 209)
(104 22) (105 11) (109 13) (110 8) (114 6)
(116 41) (117 114) (118 12) (119 15) (121 11)
(122 8) (129 164) (130 27) (133 88) (134 10)
(136 6) (137 8) (138 25) (139 35) (140 13)
(143 14) (144 6) (145 11) (147 428) (148 69)
(149 84) (150 14) (156 4) (157 35) (163 21)
(164 9) (169 34) (170 7) (171 5) (175 7)
(177 6) (185 11) (186 8) (187 36) (188 11)
(189 35) (190 11) (191 29) (192 7) (193 14)
(203 25) (205 78) (206 17) (213 14) (215 4)
(217 257) (218 59) (219 28) (220 13) (221 29)
(222 11) (228 8) (229 7) (243 27) (245 5)
(246 4) (256 6) (257 7) (260 6) (263 8)
(275 8) (276 5) (277 11) (281 4) (284 5)
(291 5) (294 3) (297 6) (298 7) (303 17)
(304 5) (305 5) (307 35) (308 12) (313 10)
(316 7) (317 9) (318 4) (319 32) (320 13)
(321 9) (322 3) (324 4) (325 4) (332 5)
(333 4) (334 7) (335 6) (336 4) (338 4)
(339 3) (340 5) (341 8) (342 7) (344 6)
(353 6) (360 6) (365 4) (366 7) (367 8)
(375 5) (377 4) (378 4) (380 4) (387 5)
(404 4) (420 6) (426 4) (432 4) (438 6)
(442 4) (443 4) (447 6) (453 4) (461 3)
(463 6) (469 8) (474 4) (477 7) (489 4)
(492 5) (511 5) (520 3) (538 3) (539 5)
(544 3) (547 4) (566 3)

NAME:12C_1682.1_1160EC15_Asparagine (3TMS)
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:168001-10-1
RI:1682
RT:10.676
NUM PEAKS: 96
(70 21) (71 6) (72 41) (73 1000) (74 132)
(75 279) (76 21) (77 24) (78 3) (79 6)
(84 10) (85 6) (86 15) (87 7) (88 4)
(89 9) (90 8) (91 3) (98 13) (99 7)
(100 120) (101 15) (102 15) (103 48) (104 5)

(105 5)	(113 4)	(114 26)	(115 33)	(116 427)
(117 60)	(118 23)	(119 6)	(125 10)	(126 3)
(127 3)	(128 21)	(129 10)	(130 34)	(131 75)
(132 209)	(133 65)	(134 15)	(135 5)	(140 3)
(141 119)	(142 23)	(143 13)	(144 16)	(145 4)
(146 8)	(147 161)	(148 28)	(149 25)	(150 3)
(156 3)	(158 6)	(159 48)	(160 10)	(161 4)
(163 3)	(169 8)	(172 12)	(173 4)	(174 9)
(188 122)	(189 27)	(190 18)	(191 4)	(199 4)
(202 36)	(203 9)	(204 14)	(205 5)	(206 3)
(213 3)	(214 3)	(215 17)	(216 11)	(217 20)
(218 37)	(219 8)	(220 4)	(229 3)	(231 147)
(232 33)	(233 14)	(243 8)	(244 4)	(245 3)
(258 25)	(259 7)	(307 5)	(316 4)	(333 7)
(348 7)				

NAME:12C_1653.8_1191EC10_[548; Leucine (2TBS)]
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:165002-10-1
RT:1654
RT:10.407
NUM PEAKS: 176

(72 23)	(73 1000)	(74 85)	(81 6)	(82 9)
(84 5)	(86 16)	(87 5)	(88 3)	(89 12)
(90 6)	(93 12)	(94 4)	(97 3)	(100 73)
(101 9)	(102 8)	(103 6)	(105 4)	(107 6)
(109 6)	(110 9)	(112 17)	(114 36)	(115 5)
(121 3)	(122 3)	(125 3)	(126 19)	(128 6)
(130 33)	(131 24)	(132 11)	(133 37)	(135 8)
(137 3)	(138 3)	(140 16)	(141 5)	(142 37)
(143 6)	(144 5)	(146 17)	(147 80)	(148 12)
(149 12)	(150 5)	(152 3)	(153 8)	(154 5)
(155 4)	(157 6)	(158 7)	(159 4)	(160 11)
(161 7)	(163 13)	(164 25)	(165 10)	(167 5)
(170 6)	(171 4)	(172 63)	(173 14)	(174 27)
(178 5)	(179 30)	(181 3)	(185 3)	(186 11)
(187 4)	(188 3)	(193 4)	(194 3)	(198 7)
(199 5)	(200 120)	(201 32)	(202 11)	(203 3)
(211 3)	(213 8)	(214 5)	(215 3)	(216 18)
(217 11)	(218 3)	(220 4)	(225 6)	(227 7)
(236 3)	(241 3)	(243 8)	(245 3)	(249 3)
(252 16)	(253 8)	(254 3)	(268 8)	(270 3)
(271 7)	(272 4)	(281 7)	(285 3)	(289 3)
(296 9)	(298 5)	(301 6)	(302 6)	(305 3)
(310 3)	(311 4)	(313 3)	(314 4)	(315 70)
(316 22)	(317 12)	(321 4)	(329 5)	(330 8)
(331 3)	(337 3)	(338 7)	(342 3)	(345 7)
(346 4)	(347 3)	(354 3)	(357 3)	(359 3)
(364 3)	(365 3)	(366 4)	(367 4)	(371 5)
(376 3)	(377 4)	(378 3)	(382 4)	(386 3)
(390 3)	(391 3)	(393 3)	(394 3)	(407 3)
(409 4)	(412 5)	(417 4)	(418 3)	(419 3)
(424 3)	(435 3)	(436 5)	(440 4)	(441 3)
(448 3)	(453 5)	(462 3)	(463 3)	(480 3)
(483 3)	(484 5)	(495 3)	(498 3)	(499 4)
(507 3)	(511 3)	(513 3)	(522 3)	(533 3)
(543 3)	(545 5)	(546 4)	(549 3)	(557 3)
(563 3)				

NAME:12C_1509.3_1178EC16_[622; Parabanic acid (2TMS)]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:151002-10-1
RI:1509
RT:9.317
NUM PEAKS: 26
(79 86) (100 1000) (101 75) (102 56) (115 834)
(116 156) (128 479) (131 79) (144 20) (153 13)
(158 66) (171 52) (201 43) (202 15) (207 39)
(243 342) (244 68) (245 30) (257 6) (261 12)
(431 6) (457 4) (518 9) (523 10) (544 7)
(568 7)

NAME:12C_1481.5_1160EC15_[815; (E)-4-Methyl-5-hydroxy-3-penten-2-one (1TMS)]
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:148002-10-1
RI:1482
RT:9.067
NUM PEAKS: 16
(72 9) (73 424) (74 52) (76 48) (82 21)
(84 43) (100 70) (112 5) (139 175) (147 54)
(148 11) (155 1000) (156 183) (229 28) (372 15)
(526 18)

NAME:12C_1467.9_1178EC16_[709; 2,5-Diaminovalerolactam (2TMS)]
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:147003-10-1
RI:1468
RT:8.883
NUM PEAKS: 105
(70 239) (71 24) (72 70) (73 1000) (74 128)
(75 164) (76 13) (77 11) (80 13) (82 16)
(83 8) (84 33) (85 20) (86 85) (87 21)
(88 12) (89 11) (95 12) (96 10) (97 11)
(98 35) (99 20) (100 413) (101 52) (102 47)
(103 14) (104 3) (105 5) (106 5) (110 11)
(111 5) (112 22) (113 32) (114 45) (115 449)
(116 64) (117 31) (118 6) (119 4) (124 4)
(125 4) (126 38) (127 21) (128 682) (129 87)
(130 52) (131 70) (132 21) (133 35) (134 6)
(135 3) (137 12) (138 3) (139 4) (140 15)
(141 292) (142 91) (143 23) (144 20) (145 3)
(146 12) (147 200) (148 33) (149 16) (152 6)
(153 56) (154 35) (155 18) (156 15) (157 5)
(158 16) (159 4) (160 4) (167 5) (168 11)
(169 145) (170 26) (171 22) (172 11) (173 3)
(174 71) (175 13) (176 5) (185 4) (186 5)
(187 4) (188 8) (200 4) (203 20) (204 4)
(214 3) (215 12) (216 26) (217 6) (227 4)
(229 8) (230 3) (241 6) (242 3) (243 199)
(244 43) (245 17) (257 4) (258 20) (259 5)

NAME:12C_1474.4_1191EC10_[NA]
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:147002-10-1
RI:1474
RT:8.933
NUM PEAKS: 136
(70 1000) (71 77) (72 122) (74 33) (75 427)
(76 48) (77 13) (78 14) (79 3) (82 5)

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( 84  123) ( 86   74) ( 87   13) ( 88   11) ( 89    3)
( 90   51) ( 91    6) ( 92    4) ( 94    4) ( 95    3)
( 97   18) ( 98   68) (100   79) (101   40) (102   14)
(103   11) (104    7) (105    6) (106    4) (107    3)
(111    5) (114   17) (115   31) (116   14) (117   27)
(118    6) (119    4) (122    3) (129    9) (130   28)
(131   27) (132   25) (133   61) (134   14) (135   10)
(136    3) (140    4) (142  100) (143   24) (144   11)
(146    7) (147   14) (148   17) (149   17) (150    6)
(151    4) (153    3) (157    7) (158   12) (159   34)
(160   16) (161    4) (163    3) (164    3) (167    4)
(168    3) (169    3) (170    5) (171   21) (172    8)
(173    5) (174   23) (175    8) (176    6) (184    3)
(185    9) (186    7) (188    7) (190    5) (197    3)
(200    3) (203    4) (204    6) (211    6) (212    3)
(213    3) (216    4) (217    7) (218   65) (219   16)
(220    8) (230    4) (236    7) (240    3) (241    7)
(242    3) (248    8) (256    6) (259    7) (260    5)
(261    4) (273    3) (275    3) (276   12) (277    5)
(292   10) (293    7) (294    4) (305    3) (307    3)
(319    3) (320   15) (321    6) (322    4) (336    3)
(353    4) (354    4) (362    3) (372    3) (376    3)
(407    3) (408    3) (421    3) (422    3) (428    3)
(429    3) (430    3) (435    3) (436    3) (444    3)
(464    3) (465    3) (478    3) (483    3) (490    3)
(494    3)
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NAME:12C_1296.5_1191EC10_Phosphoric acid (3TMS)
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:129001-10-1
RI:1297
RT:6.913
NUM PEAKS:  89
( 70    7) ( 71   11) ( 72   26) ( 73 1000) ( 74  106)
( 75   97) ( 76    5) ( 77   37) ( 79    6) ( 84    3)
( 85    7) ( 87   12) ( 88    4) ( 89   19) ( 91   10)
(102    5) (103   83) (104   13) (105   28) (106    4)
(107   15) (109    5) (113    3) (115   53) (116   11)
(119   39) (120    6) (121   22) (122    3) (123   10)
(131   36) (132    8) (133  250) (134   34) (135   68)
(136    8) (137   35) (138    4) (139    3) (145    4)
(150    4) (151   23) (152    3) (153    5) (163    8)
(165   13) (166    4) (167   13) (176    3) (177   11)
(178    4) (179    9) (180    3) (181   36) (182    6)
(183   13) (184    3) (189   13) (190    4) (191   50)
(192   12) (193   53) (194   10) (195   14) (196    3)
(197    4) (207   54) (208   11) (209    9) (210    3)
(211  128) (212   19) (213   10) (221    5) (225   24)
(226    5) (227    7) (269    4) (283   24) (284    9)
(285    4) (298    8) (299  436) (300  112) (301   58)
(302   10) (314   62) (315   16) (316    8)
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NAME:12C_1220.2_1274EC17_Valine (2TMS)
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:122001-10-1
RI:1220
RT:6.122
NUM PEAKS:  55
( 70   15) ( 71    6) ( 72   60) ( 73  846) ( 74   82)
( 75   98) ( 76    7) ( 77    4) ( 82    6) ( 83    4)
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( 84    4) ( 85    5) ( 86   13) ( 87    5) ( 98    4)
( 99    4) (100  114) (101   16) (102    9) (103   24)
(104    3) (105    3) (112    4) (114    9) (115    7)
(116    3) (117   11) (118    3) (119    3) (128   19)
(129   12) (130   12) (131   15) (132   17) (133   26)
(134    4) (142    6) (143    5) (144 1000) (145  134)
(146   49) (147  153) (148   24) (149   14) (156   22)
(157    4) (158    3) (160    3) (163    4) (174    4)
(203    3) (218  143) (219   34) (220   13) (246    9)

NAME:12C_1282.1_1274EC17_Serine (2TMS)
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:128001-10-1
RI:1282
RT:6.820
NUM PEAKS:  62
( 70   19) ( 71    6) ( 72   25) ( 73  961) ( 74  123)
( 75  316) ( 76   31) ( 81   15) ( 84    3) ( 85    6)
( 86   71) ( 87   24) ( 88   36) ( 89   16) ( 90    6)
( 91   10) ( 96    4) ( 98    4) ( 99    5) (100  110)
(101   24) (102   29) (103  134) (104   14) (105    7)
(114    8) (115    9) (116 1000) (117  112) (118   43)
(119    6) (128    3) (130   71) (131   37) (132  761)
(133  118) (134   35) (142    3) (143    4) (144  134)
(145   16) (146   76) (147   99) (148   19) (149   15)
(159   57) (160    8) (161    4) (172    3) (188   17)
(189    5) (190    4) (206    5) (216    5) (217    4)
(219   33) (220    7) (221    3) (234   31) (235    7)
(236    3) (262    3)

NAME:12C_1326.5_1274EC17_Glycine (3TMS)
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:133001-10-1
RI:1327
RT:7.320
NUM PEAKS:  48
( 71    4) ( 72   14) ( 73  561) ( 74   44) ( 85    4)
( 86  340) ( 87   29) ( 88   13) ( 99    3) (100  189)
(101   30) (102   23) (103   10) (105    3) (113    5)
(115    4) (116    7) (119    8) (131   21) (133   99)
(134   14) (135    7) (144    6) (147  290) (148   46)
(149   23) (158    7) (159    3) (160   21) (161    4)
(172   10) (173    3) (174 1000) (175  189) (176   83)
(177   18) (188    8) (202    3) (204    4) (246   11)
(247    4) (248  139) (249   42) (250   19) (251    3)
(276   52) (277   14) (278    7)

NAME:12C_1352.5_1274EC17_Glyceric acid (3TMS)
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:135003-10-1
RI:1353
RT:7.614
NUM PEAKS:  78
( 70   47) ( 71  197) ( 72   20) ( 73 1000) ( 74   74)
( 82   11) ( 83   10) ( 84   28) ( 85   99) ( 89    9)
( 97    3) ( 99   22) (101   28) (102  169) (103  170)
(104   20) (105    8) (106    4) (109    5) (111    6)
(113   21) (115   12) (116   11) (117   88) (118    6)
(119   11) (124    4) (125    3) (126   10) (127   16)
(130   66) (131   35) (133  169) (141    3) (145    4)
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(147 458) (148 54) (149 23) (152 3) (155 7)
(162 4) (163 7) (168 5) (169 13) (173 4)
(175 9) (177 8) (179 3) (188 3) (189 311)
(190 50) (191 27) (196 7) (204 10) (205 64)
(206 9) (207 7) (212 6) (216 4) (217 16)
(221 30) (222 10) (226 14) (236 4) (241 4)
(249 3) (251 3) (256 7) (267 18) (268 8)
(278 4) (281 10) (292 100) (293 31) (294 10)
(297 3) (306 3) (307 25)

NAME:12C_1394.9_1274EC17_[644; 2-Methyl-1,3-butanediol (2TMS)]
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:140003-10-1
RI:1395
RT:8.092
NUM PEAKS: 50
(71 81) (72 29) (73 1000) (74 85) (75 259)
(76 23) (101 43) (102 7) (115 29) (116 193)
(117 836) (118 85) (119 39) (129 20) (130 5)
(131 33) (133 123) (134 25) (143 175) (144 47)
(145 33) (147 405) (148 67) (149 140) (150 15)
(163 9) (175 16) (176 6) (189 5) (203 31)
(204 7) (217 21) (221 15) (233 62) (234 98)
(235 25) (236 8) (245 30) (246 9) (291 6)
(293 4) (299 5) (305 6) (306 107) (307 36)
(308 18) (309 5) (335 11) (389 4) (405 5)

NAME:12C_1403.1_1274EC17_Threonine (3TMS)
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:140001-10-1
RI:1403
RT:8.183
NUM PEAKS: 98
(71 5) (72 23) (73 1000) (74 93) (75 109)
(76 8) (84 10) (85 7) (86 19) (87 19)
(88 6) (89 15) (98 5) (99 5) (100 93)
(101 187) (102 29) (104 4) (105 8) (106 2)
(112 4) (113 3) (114 22) (115 22) (116 9)
(117 303) (118 34) (119 27) (120 3) (128 70)
(129 88) (130 53) (131 50) (132 46) (133 71)
(134 17) (135 22) (142 3) (144 6) (145 4)
(146 13) (147 176) (148 31) (149 21) (150 4)
(156 3) (158 7) (159 9) (160 9) (161 3)
(163 8) (165 3) (172 6) (174 6) (175 3)
(176 4) (177 7) (178 3) (186 5) (188 4)
(189 5) (190 4) (191 18) (192 13) (193 14)
(202 25) (203 28) (204 12) (206 5) (207 23)
(208 12) (209 5) (212 2) (216 4) (217 3)
(218 211) (219 239) (220 57) (224 20) (226 4)
(230 7) (231 3) (240 8) (244 2) (248 2)
(269 4) (282 14) (283 6) (284 3) (291 56)
(292 35) (293 14) (294 5) (316 2) (320 10)
(321 5) (329 5) (344 5)

NAME:12C_1414.0_1274EC17_[590; 1-Acetyl-2-thiohydantoin]
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:141004-10-1
RI:1414
RT:8.306
NUM PEAKS: 71

(70	11)	(72	79)	(73	774)	(74	215)	(75	1000)
(76	99)	(77	76)	(78	6)	(79	12)	(80	3)
(82	9)	(83	53)	(84	39)	(85	11)	(86	28)
(87	37)	(88	13)	(89	17)	(90	4)	(91	19)
(92	3)	(93	14)	(95	5)	(98	40)	(99	10)
(100	29)	(101	107)	(102	29)	(103	72)	(104	8)
(105	30)	(106	3)	(112	16)	(113	10)	(114	117)
(115	20)	(116	756)	(117	246)	(118	30)	(119	11)
(126	4)	(128	17)	(129	50)	(130	521)	(131	67)
(132	24)	(140	24)	(141	4)	(142	8)	(143	10)
(144	23)	(145	7)	(146	104)	(148	73)	(149	9)
(150	3)	(156	29)	(157	12)	(158	278)	(159	35)
(160	14)	(172	7)	(173	37)	(174	9)	(176	22)
(190	7)	(191	3)	(200	13)	(215	4)	(218	6)
(233	3)								

NAME:12C_1440.3_1274EC17_[678; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:144003-10-1
RI:1440
RT:8.603
NUM PEAKS: 63

(70	58)	(71	6)	(72	32)	(73	1000)	(74	117)
(75	312)	(76	30)	(77	16)	(84	4)	(85	4)
(86	10)	(87	8)	(88	6)	(89	8)	(91	5)
(98	6)	(99	7)	(100	53)	(101	11)	(102	21)
(103	13)	(115	7)	(116	223)	(117	264)	(118	36)
(119	12)	(128	17)	(129	7)	(130	310)	(131	48)
(132	20)	(133	24)	(134	4)	(135	3)	(143	3)
(144	43)	(145	6)	(146	27)	(147	133)	(148	24)
(149	18)	(150	3)	(159	25)	(160	581)	(161	73)
(162	26)	(172	10)	(174	6)	(187	7)	(190	3)
(202	21)	(203	4)	(220	16)	(221	3)	(234	33)
(235	8)	(236	3)	(244	7)	(245	50)	(246	11)
(247	4)	(262	17)	(263	3)				

NAME:12C_1488.2_1274EC17_Malic acid (3TMS)
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:149001-10-1
RI:1488
RT:9.143
NUM PEAKS: 79

(70	7)	(72	30)	(73	1000)	(74	84)	(75	146)
(76	13)	(77	12)	(78	3)	(82	5)	(83	3)
(84	47)	(87	6)	(93	5)	(99	6)	(101	77)
(102	8)	(103	13)	(105	5)	(111	3)	(115	10)
(116	12)	(117	53)	(118	6)	(119	9)	(129	10)
(131	35)	(132	6)	(133	126)	(134	17)	(135	12)
(143	21)	(144	5)	(145	5)	(146	3)	(147	505)
(148	76)	(149	48)	(150	4)	(151	6)	(171	24)
(172	4)	(173	4)	(175	48)	(176	8)	(177	13)
(185	3)	(189	63)	(190	48)	(191	40)	(192	9)
(193	3)	(203	5)	(205	3)	(217	25)	(218	6)
(219	3)	(221	12)	(222	3)	(233	112)	(234	22)
(235	8)	(245	66)	(246	12)	(247	8)	(260	3)
(263	14)	(264	4)	(265	20)	(266	4)	(305	4)
(306	7)	(307	21)	(308	9)	(309	4)	(319	5)
(320	3)	(335	26)	(336	6)	(337	4)		

NAME:12C_1565.1_1274EC17_Phenylalanine (1TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:157001-10-1
RI:1565
RT:9.777
NUM PEAKS: 49

(72 4)	(73 277)	(74 82)	(75 218)	(76 24)
(77 75)	(78 12)	(79 3)	(80 3)	(86 17)
(87 14)	(88 4)	(89 14)	(90 8)	(91 163)
(92 29)	(93 28)	(94 3)	(100 6)	(102 15)
(103 105)	(104 17)	(105 4)	(116 3)	(117 10)
(118 42)	(119 26)	(120 1000)	(121 96)	(122 3)
(130 233)	(131 38)	(132 9)	(146 460)	(147 48)
(148 19)	(149 3)	(160 3)	(161 3)	(176 11)
(177 14)	(178 3)	(194 10)	(204 37)	(205 11)
(206 3)	(222 30)	(223 5)	(237 3)	

NAME:12C_1573.9_1274EC17_[708; 2,3-Dimethylsuccinic acid (2TMS)]
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:157002-10-1
RI:1574
RT:9.844
NUM PEAKS: 85

(70 9)	(71 25)	(72 20)	(73 1000)	(74 85)
(75 205)	(76 13)	(77 7)	(81 5)	(83 21)
(85 16)	(87 3)	(89 9)	(95 9)	(97 45)
(98 7)	(99 17)	(101 7)	(102 3)	(103 14)
(110 3)	(111 6)	(113 9)	(115 5)	(117 49)
(119 4)	(127 5)	(131 22)	(132 3)	(133 81)
(134 12)	(135 9)	(141 5)	(143 141)	(144 17)
(145 9)	(147 442)	(148 69)	(149 88)	(150 10)
(151 4)	(157 71)	(158 11)	(161 8)	(169 5)
(171 9)	(177 11)	(184 3)	(185 5)	(189 3)
(190 5)	(191 156)	(192 27)	(193 12)	(213 16)
(217 21)	(218 3)	(220 5)	(221 15)	(222 3)
(231 47)	(232 11)	(233 7)	(243 18)	(244 3)
(245 5)	(259 4)	(265 38)	(266 10)	(267 3)
(275 128)	(276 30)	(277 11)	(287 15)	(288 3)
(289 3)	(299 3)	(305 16)	(306 6)	(307 3)
(349 5)	(350 3)	(377 20)	(378 8)	(379 3)

NAME:12C_1581.5_1274EC17_[680; 2,3-Dimethylsuccinic acid (2TMS)]
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:158003-10-1
RI:1582
RT:9.903
NUM PEAKS: 109

(70 11)	(71 120)	(72 29)	(73 1000)	(74 88)
(75 251)	(76 17)	(77 11)	(81 5)	(83 4)
(85 8)	(87 6)	(89 4)	(91 37)	(92 4)
(93 3)	(95 21)	(96 4)	(97 24)	(99 11)
(101 7)	(102 3)	(103 12)	(105 4)	(113 61)
(114 5)	(115 66)	(116 10)	(117 70)	(118 7)
(119 9)	(123 11)	(127 5)	(129 38)	(130 5)
(131 40)	(132 7)	(133 80)	(134 11)	(135 9)
(141 14)	(142 3)	(143 43)	(144 7)	(145 6)
(147 493)	(148 78)	(149 95)	(150 13)	(151 6)
(157 108)	(158 18)	(159 8)	(161 3)	(163 20)
(164 3)	(169 18)	(170 3)	(171 10)	(173 4)
(175 4)	(177 3)	(185 50)	(186 9)	(187 5)
(189 12)	(190 6)	(191 10)	(197 4)	(203 5)

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(204     5) (205     4) (207     4) (212     4) (213    49)
(214     8) (215     5) (217    37) (218     8) (219     6)
(221    20) (222     5) (223     3) (231    62) (232    19)
(233    10) (243     6) (245     6) (259    62) (260    16)
(261    28) (262     6) (275   233) (276    57) (277    26)
(278     4) (287    47) (288    11) (289     6) (305    11)
(306     4) (307     4) (333     3) (349    36) (350    16)
(351     8) (377    37) (378    13) (379     6)
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NAME:12C_1595.8_1274EC17_[639; Proline (2TMS)]
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:159001-10-1
RI:1596
RT:10.013
NUM PEAKS:  51
( 70    29) ( 72    85) ( 73  1000) ( 74    92) ( 75    92)
( 78     5) ( 86    12) ( 87     5) ( 89     3) ( 96     6)
( 98     8) ( 99    26) (100    19) (101     9) (102     6)
(105     8) (106     3) (107     4) (113     6) (115     6)
(116     5) (119     3) (126     7) (129     6) (131    19)
(132     3) (133    37) (134     4) (140     8) (142   829)
(143   112) (144    32) (147   203) (148    30) (149    13)
(170    15) (171     4) (172     6) (186   681) (187    95)
(188    27) (193     4) (216   126) (217    34) (218    11)
(244     9) (288    65) (289    15) (290     6) (303    10)
(304     3)
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NAME:12C_1625.9_1274EC17_Glutamic acid (3TMS)
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:163001-10-1
RI:1626
RT:10.245
NUM PEAKS:  104
( 70     9) ( 71     5) ( 72    36) ( 73  1000) ( 74   108)
( 75   342) ( 76    18) ( 77     8) ( 82     7) ( 83     9)
( 84   343) ( 85    26) ( 86    12) ( 87     8) ( 88     3)
( 89     5) ( 95     6) ( 96     3) ( 98    10) ( 99     4)
(100    97) (101    19) (102    10) (103    11) (112    13)
(113    11) (114    22) (115    21) (116     4) (117    23)
(118     3) (119     7) (126     3) (128   392) (129    67)
(130    31) (131    31) (132    23) (133    68) (134    10)
(140    45) (141     7) (142     6) (143     6) (144     6)
(145     5) (146     7) (147   263) (148    44) (151     3)
(154     4) (155     4) (156   255) (157    45) (158    61)
(159     3) (160     5) (163     4) (172     5) (173     6)
(174    57) (175     7) (186    11) (188     4) (189     5)
(191     3) (198     3) (201     3) (202     8) (203     6)
(204    33) (205     7) (206     4) (214    10) (215     4)
(216     6) (218    35) (219    10) (220     4) (221    12)
(229     3) (230   117) (231    28) (232    13) (245    11)
(246   695) (247   149) (248    63) (249     8) (258    19)
(259     5) (260     3) (273     3) (274     6) (276     5)
(299     4) (320     6) (321     3) (348    32) (349    10)
(350     5) (363    15) (364     6) (365     3)
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NAME:12C_1770.3_1274EC17_[NA]
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:177003-10-1
RI:1770
RT:11.356
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NUM PEAKS:  52
( 82    47) ( 84    40) ( 86   615) (100   394) (112    34)
(125    11) (126     8) (128    12) (140    40) (141     4)
(144    60) (156   194) (157    32) (158   136) (160    21)
(169     5) (170     4) (171     5) (172   796) (173   278)
(174  1000) (175   157) (176    61) (185    40) (187    27)
(199   262) (200    86) (201    27) (202    12) (214    38)
(215    10) (217    14) (230     9) (231     5) (239    41)
(244   157) (245    27) (246    50) (247     3) (273    21)
(274     6) (305     4) (329    87) (330   206) (331    89)
(332    34) (345   165) (346    64) (347    22) (361    16)
(362    13) (363     5)
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NAME:12C_1794.4_1274EC17_[789; Tyramine (3TMS)]
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:179002-10-1
RI:1794
RT:11.541
NUM PEAKS:  53
( 72     9) ( 73   612) ( 74    57) ( 75   158) ( 76     8)
( 86   350) ( 87    23) ( 88     4) ( 89    93) ( 90     4)
(100   127) (101    19) (102    38) (105     4) (117    19)
(118     5) (128     6) (129    39) (130    48) (131     9)
(144     6) (146    27) (147     4) (148     6) (156    12)
(160    29) (161     4) (167     7) (174  1000) (175   185)
(176    78) (183     6) (190    70) (191     7) (199    10)
(217     3) (223    14) (230     3) (231     7) (238     4)
(239     3) (244     3) (246     7) (255     5) (260     3)
(287     4) (331     4) (345    80) (346    30) (347    10)
(348     3) (361    16) (362     6)
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NAME:12C_1806.4_1274EC17_[944; D-Mannopyranose (5TMS)]
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:181005-10-1
RI:1806
RT:11.634
NUM PEAKS:  148
( 70    12) ( 72     7) ( 73  1000) ( 74    88) ( 75    73)
( 81    23) ( 83    24) ( 87     9) ( 89    28) ( 93    10)
( 94     5) ( 95     4) ( 96     7) ( 97    26) ( 98     5)
(103    56) (105    10) (106     8) (108     4) (109     5)
(110     3) (111    15) (112     3) (116     3) (117    81)
(118     6) (120     4) (123     4) (125    13) (129   109)
(130    20) (131    35) (132     5) (133    56) (134     8)
(137     4) (143    23) (145     7) (147   201) (148    42)
(149    27) (150     5) (152     6) (153     3) (157    17)
(161     5) (165     4) (166     4) (169     7) (170     3)
(171     5) (175    10) (187     3) (189    56) (190    19)
(191   567) (192    97) (193    40) (194    15) (203    22)
(204   839) (205   159) (206    66) (207    14) (209     5)
(210     5) (217   141) (218    37) (219    16) (220     6)
(221     8) (222     8) (223     6) (230     5) (231    22)
(232     5) (233     6) (234     4) (237    18) (238     7)
(243    13) (244     3) (245     4) (250     4) (252     3)
(253     3) (258     3) (259     4) (264     3) (265     8)
(271     6) (272     3) (279     7) (284     3) (290     3)
(291    10) (292     6) (298     3) (305    15) (306     8)
(307     4) (312    13) (317     8) (319     3) (323     5)
(325     4) (327     3) (333     3) (345    13) (346     3)
(367     5) (368     8) (369     4) (370     5) (384     3)
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(393    7) (394    5) (397    4) (398    3) (403    4)
(404    4) (413    4) (423    6) (426    4) (434    6)
(435   10) (437    4) (438    5) (439    3) (458    6)
(463    5) (473    4) (474    4) (475    4) (479    3)
(485    8) (489    3) (490    4) (493    4) (498    5)
(519    3) (526    5) (527    5) (541    3) (549    5)
(553    4) (560    4) (570    4)
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NAME:12C_1868.5_1274EC17_[826; beta-[[(5-methyl-2-thienyl)methylene]amino]-
benzeneacetic acid methyl ester]
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:187004-10-1
RI:1869
RT:12.112
NUM PEAKS:  78
( 70    8) ( 71    7) ( 72   14) ( 73  962) ( 74   77)
( 75   59) ( 80    3) ( 81    9) ( 85    5) ( 93    4)
( 95    6) ( 97    3) ( 98   11) ( 99    5) (101   12)
(115    3) (116    7) (118    3) (119    6) (124    4)
(125    4) (126    3) (131   16) (133   46) (135    5)
(138    4) (139    3) (140    3) (141    3) (147  102)
(148   19) (149   11) (151    8) (153   72) (154   18)
(155    6) (165    4) (166    5) (167   51) (168    9)
(169  110) (170   71) (171   13) (179    4) (181    3)
(183    6) (184    3) (195    8) (197    4) (198    3)
(204   15) (210    5) (211   10) (212   10) (213    3)
(225    4) (226   11) (227    6) (239   20) (240    9)
(241 1000) (242  248) (243   96) (244   13) (267   13)
(268    4) (269    4) (284    4) (315    6) (341    3)
(343    3) (356    6) (374    3) (431   18) (432    9)
(433    4) (446    5) (447    3)
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NAME:12C_1877.4_1274EC17_alpha-D-Methylglucopyranoside (4TMS)
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:188006-10-1
RI:1877
RT:12.180
NUM PEAKS:  207
( 70  203) ( 73 1000) ( 74  100) ( 81   19) ( 85   13)
( 87   16) ( 89   35) ( 90    6) ( 98    7) (100   16)
(101   40) (107    5) (109    8) (113    9) (116   23)
(117   30) (118    6) (119    7) (124    4) (125    4)
(131   41) (133  338) (134   37) (135    9) (136    4)
(143   14) (144    4) (146   41) (152    3) (155   10)
(159   19) (163   12) (164    4) (166    4) (177    5)
(183   10) (184    3) (185    6) (189   14) (190   12)
(191   35) (192    5) (193    6) (197    5) (203   24)
(204  500) (206   34) (207    6) (208    6) (209    4)
(213    7) (215    5) (217   66) (218   23) (219   10)
(222    5) (227    4) (228    4) (231   15) (233   12)
(234    6) (236    2) (237    2) (239    3) (243    8)
(244    5) (245    4) (247    6) (250    4) (251    4)
(253    2) (255    3) (256    4) (261    4) (265    7)
(266    5) (270    3) (271    7) (272    5) (273    3)
(274    3) (280    3) (286    7) (287    9) (288    6)
(289    5) (290   18) (291   14) (293    4) (295    3)
(296    6) (297    4) (298    7) (299   20) (303    9)
(305   10) (306   10) (313    6) (314    5) (315    6)
(317   12) (318    4) (324    4) (325    6) (327    3)
(332    5) (333    6) (334    3) (335    5) (336    3)
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(337    6) (338    3) (341    4) (345    4) (349    4)
(353    4) (361    7) (371    3) (372    2) (374    3)
(376    3) (377    6) (381    3) (382    3) (385    2)
(386    7) (387    4) (388    5) (391    5) (393    4)
(396    4) (399    4) (400    3) (405    3) (408    3)
(409    4) (412    3) (413    3) (414    6) (415    5)
(429    3) (430    4) (431    3) (436    4) (437    9)
(438    8) (439    4) (446    4) (448    4) (450    2)
(451    5) (454    3) (456    3) (457    4) (461    2)
(464    5) (469    6) (472    4) (473    5) (476    4)
(477    3) (478    3) (480    4) (482    6) (485    3)
(486    5) (489    5) (490    5) (491    4) (495    5)
(496    5) (497    4) (501    7) (503    6) (507    5)
(508    3) (510    4) (511    6) (514    6) (515    5)
(517    5) (518    3) (521    6) (524    4) (526    3)
(529    7) (533    4) (535    3) (536    3) (538    4)
(539    5) (541    4) (547    6) (548    3) (549    3)
(553    3) (557    4) (559    3) (563    4) (565    2)
(567    2) (568    2) (569    2) (574    2) (576    2)
(578    2) (584    2)

NAME:12C_1889.9_1274EC17_Glucose methoxyamine (5TMS)
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:189002-10-1
RI:1890
RT:12.276
NUM PEAKS:  137
( 70    5) ( 71    6) ( 72   20) ( 73 1000) ( 83   24)
( 86    6) ( 89   55) ( 98    3) ( 99    6) (100   19)
(101   20) (102    9) (103  143) (104    7) (105   24)
(110    4) (111    3) (112    3) (113    6) (114   16)
(115    6) (117  112) (126    2) (127    5) (128    7)
(129  168) (131   30) (133   96) (134   10) (140    2)
(141    3) (142    9) (143   20) (144    3) (145    6)
(147  426) (148   69) (154    2) (155    2) (156    2)
(157  150) (158   27) (159   10) (160  222) (161   41)
(162    9) (168    3) (169    3) (170    2) (171    1)
(172    6) (173    7) (174   12) (184    1) (185    2)
(186    6) (187    3) (188    2) (189   43) (190   11)
(196    1) (198    2) (200    5) (201   12) (202    4)
(203    6) (205  274) (206   54) (207   22) (214    2)
(215    4) (216   12) (217  141) (218   22) (221    5)
(222    2) (228    2) (229   39) (230   14) (231   16)
(232    8) (233   11) (234    6) (235    2) (240    3)
(241    1) (242    2) (243    3) (244    6) (245    3)
(246    6) (247    3) (248    2) (254    1) (255    1)
(256    3) (257    2) (259    2) (260    2) (261    2)
(262    7) (263    2) (268    2) (269    3) (270    3)
(271    1) (272    1) (274    7) (275    3) (276    2)
(277    7) (278    3) (279    1) (291   12) (300    4)
(302    1) (305    9) (306    4) (307    7) (318    7)
(319  253) (320   81) (321   38) (322    8) (323    2)
(330    1) (332    1) (333    1) (343    2) (344    2)
(364    4) (365    3) (366    1) (374    3) (375    1)
(376    2) (464    1)

NAME:12C_1909.6_1274EC17_Glucose methoxyamine (BP) (5TMS)
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:191001-10-1
RI:1910
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RT:12.415
NUM PEAKS:  65
( 72    6) ( 73 1000) ( 74   77) ( 75   66) ( 76    3)
( 89   62) ( 90    3) ( 91    3) (101   11) (103  186)
(104   17) (105   23) (116    4) (117   84) (118    7)
(119    8) (129  127) (130    8) (131   23) (133   83)
(134   10) (135    6) (143   12) (145    3) (147  304)
(148   42) (149   28) (150    3) (157   97) (158   11)
(159    8) (160  134) (161   27) (162    7) (163   12)
(177    6) (189   30) (190   24) (191   15) (201    6)
(203    3) (204   24) (205  195) (206   41) (207   21)
(214    3) (217   86) (218   16) (219    6) (221    6)
(229   27) (233   16) (234    4) (235    6) (243    3)
(277    9) (278    5) (291    7) (300    3) (305    4)
(307    5) (319  183) (320   57) (321   26) (322    5)

NAME:12C_1915.4_1274EC17_Lysine (4TMS)
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:192003-10-1
RI:1915
RT:12.451
NUM PEAKS:  122
( 70   11) ( 71   10) ( 72   19) ( 73 1000) ( 74  110)
( 75   73) ( 76    5) ( 77    3) ( 82   20) ( 83    5)
( 84   36) ( 85   15) ( 86  123) ( 87   16) ( 88   57)
( 89    6) ( 90    4) ( 94    5) ( 97    3) ( 98   11)
( 99   10) (100  115) (101   17) (102   37) (103   13)
(104    3) (110    4) (112   32) (113   10) (114   34)
(115   36) (116   16) (117   22) (118    5) (119    5)
(124    3) (126   15) (127    4) (128  157) (129   24)
(130   51) (131   32) (132   23) (133   31) (134    6)
(135    3) (138    3) (139    3) (140   31) (141    8)
(142   21) (143    5) (144    7) (145    3) (146   30)
(147   98) (148   20) (149   10) (150    3) (151   10)
(152    3) (154   36) (155   19) (156  540) (157   80)
(158   34) (159    5) (160   11) (161    3) (162    3)
(166    7) (167    4) (168    7) (170    5) (172   20)
(173    5) (174  501) (175   94) (176   43) (177    5)
(179   11) (184    5) (186   14) (187    4) (188    6)
(189    4) (191   11) (200   55) (201   12) (202   17)
(203    4) (204    3) (212    4) (213    4) (214   15)
(215    7) (216    8) (218   19) (219    8) (220    5)
(228   31) (229    9) (230  118) (231   26) (232   12)
(240    3) (244    3) (255    3) (258    6) (272    6)
(273    8) (274    4) (317  110) (318   39) (319   15)
(320    3) (329   11) (330    5) (419    3) (434   12)
(435    7) (436    3)

NAME:12C_1938.9_1274EC17_Tyrosine (3TMS)
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:194002-10-1
RI:1939
RT:12.600
NUM PEAKS:  79
( 70    4) ( 72   18) ( 73 1000) ( 74   94) ( 75  108)
( 76    7) ( 77    9) ( 78    4) ( 79    3) ( 82    4)
( 84    4) ( 86   10) ( 87    8) ( 89    9) ( 90    7)
( 91   17) (100  198) (101   26) (102   12) (103   15)
(104    4) (105   10) (115    9) (116    4) (117   14)
(118    8) (119    9) (130   22) (131   30) (132   26)
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(133 32) (134 7) (135 11) (144 3) (145 4)
(146 11) (147 267) (148 47) (149 41) (150 6)
(151 5) (158 3) (159 3) (160 7) (161 5)
(162 3) (163 22) (164 8) (165 12) (174 7)
(175 5) (176 7) (177 7) (179 122) (180 28)
(181 8) (190 5) (192 16) (193 6) (203 5)
(207 7) (208 7) (218 883) (219 179) (220 79)
(221 10) (223 3) (265 9) (266 3) (279 4)
(280 68) (281 18) (282 6) (292 3) (354 14)
(355 7) (356 4) (382 8) (383 3)

NAME:12C_2023.7_1274EC17_[680; Glycerol-2-phosphate (4TMS)]
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:203004-10-1
RI:2024
RT:13.138
NUM PEAKS: 93
(70 7) (72 22) (73 1000) (74 84) (75 188)
(76 13) (77 20) (86 5) (88 14) (89 11)
(90 3) (95 16) (99 11) (101 15) (103 22)
(105 7) (111 10) (113 15) (114 4) (115 13)
(121 5) (125 4) (126 5) (127 11) (130 8)
(131 16) (133 86) (134 11) (135 23) (137 12)
(141 9) (142 10) (143 11) (147 254) (148 39)
(149 32) (150 5) (151 6) (153 10) (155 11)
(160 7) (161 5) (163 3) (167 9) (168 11)
(169 138) (170 24) (171 22) (177 3) (179 9)
(181 11) (183 8) (184 27) (185 9) (186 3)
(193 10) (195 12) (197 3) (198 4) (200 5)
(207 14) (208 5) (211 102) (212 19) (213 9)
(215 9) (225 13) (227 34) (228 7) (229 4)
(241 7) (242 3) (243 203) (244 46) (245 23)
(253 7) (256 3) (257 7) (258 115) (259 32)
(260 13) (285 4) (297 58) (298 14) (299 107)
(300 31) (301 16) (302 4) (315 93) (316 25)
(317 11) (370 4) (485 5)

NAME:12C_2029.2_1274EC17_[910; 9-(Z)-Hexadecenoic acid (1TMS)]
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:203002-10-1
RI:2029
RT:13.173
NUM PEAKS: 136
(70 37) (71 26) (72 39) (73 715) (74 83)
(75 1000) (76 70) (77 71) (78 12) (79 85)
(80 34) (81 177) (82 84) (83 121) (84 171)
(85 34) (86 11) (87 6) (88 5) (89 25)
(90 3) (91 37) (92 12) (93 53) (94 30)
(95 124) (96 197) (97 108) (98 143) (99 33)
(100 3) (101 10) (102 6) (103 3) (105 33)
(106 7) (107 26) (108 18) (109 64) (110 74)
(111 48) (112 29) (113 7) (115 6) (116 60)
(117 697) (118 68) (119 52) (120 8) (121 30)
(122 12) (123 52) (124 32) (125 16) (126 6)
(127 7) (128 5) (129 533) (130 66) (131 109)
(132 124) (133 44) (134 26) (135 19) (136 9)
(137 39) (138 33) (139 13) (140 4) (141 14)
(142 6) (143 36) (144 7) (145 211) (146 28)
(148 11) (149 6) (150 4) (151 24) (152 70)
(153 13) (154 4) (155 29) (156 9) (157 16)

(158 7) (159 18) (161 7) (162 4) (163 4)
(165 14) (166 13) (167 4) (169 3) (170 6)
(171 25) (172 10) (173 12) (174 4) (175 3)
(179 6) (180 5) (183 16) (185 49) (186 12)
(187 10) (188 5) (192 9) (193 11) (194 48)
(195 7) (199 62) (200 12) (201 12) (202 3)
(207 4) (208 7) (213 12) (214 3) (215 4)
(218 3) (227 7) (229 8) (230 3) (236 32)
(237 7) (241 4) (255 3) (267 4) (283 4)
(310 4) (311 136) (312 39) (313 9) (326 15)
(327 5)

NAME:12C_1675.0_1274EC11_[877; Pyrophosphoric acid (4TMS)]
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:168004-10-1
RI:1675
RT:10.627
NUM PEAKS: 96
(70 7) (71 12) (72 46) (73 1000) (74 92)
(75 44) (83 12) (85 8) (87 3) (89 6)
(91 4) (95 6) (97 7) (98 3) (99 5)
(100 6) (103 21) (104 5) (107 5) (111 4)
(114 3) (115 9) (119 10) (121 14) (125 3)
(127 21) (131 6) (133 61) (134 7) (135 43)
(136 4) (137 11) (139 4) (146 13) (151 9)
(165 8) (167 5) (177 5) (179 5) (180 3)
(181 10) (187 3) (189 5) (191 24) (192 7)
(193 48) (194 7) (195 28) (196 4) (197 6)
(205 5) (207 57) (208 12) (209 10) (211 10)
(212 3) (217 17) (218 5) (225 13) (226 3)
(230 3) (254 3) (255 7) (257 4) (267 3)
(269 12) (270 3) (273 3) (283 16) (284 6)
(285 26) (286 6) (297 4) (299 74) (300 18)
(301 8) (313 6) (314 7) (315 3) (362 3)
(363 24) (364 7) (365 4) (435 4) (436 4)
(449 5) (450 55) (451 369) (452 150) (453 80)
(454 21) (455 6) (465 5) (466 35) (467 15)
(468 9)

NAME:12C_1673.8_1191EC10_Homocysteine (3TMS)
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:167001-10-1
RI:1674
RT:10.561
NUM PEAKS: 223
(70 16) (72 171) (75 990) (76 88) (77 1000)
(78 54) (79 20) (82 133) (84 120) (88 18)
(89 233) (90 28) (91 61) (92 38) (93 136)
(94 11) (95 104) (97 29) (98 463) (99 39)
(101 48) (102 26) (103 326) (104 38) (105 44)
(106 5) (107 10) (111 21) (114 105) (119 83)
(120 9) (121 19) (122 13) (124 16) (125 15)
(127 136) (128 510) (129 16) (130 63) (137 15)
(139 17) (142 13) (144 40) (146 159) (155 29)
(156 89) (157 39) (161 5) (162 23) (165 19)
(166 4) (167 8) (171 49) (176 6) (183 14)
(184 22) (185 22) (187 33) (193 22) (200 14)
(201 4) (202 21) (203 14) (212 21) (214 5)
(224 6) (228 4) (229 18) (230 19) (234 191)
(235 42) (236 18) (241 5) (244 12) (250 10)

(257 10) (261 10) (262 14) (265 6) (266 7)
(267 7) (268 23) (271 30) (280 5) (281 4)
(283 11) (291 4) (293 4) (294 6) (295 10)
(298 6) (308 19) (309 4) (312 5) (314 38)
(315 12) (316 17) (318 9) (319 18) (320 9)
(322 12) (325 10) (334 19) (335 8) (337 16)
(338 7) (340 10) (345 10) (346 22) (348 6)
(349 4) (350 17) (351 14) (352 9) (353 8)
(368 4) (370 9) (371 13) (372 5) (381 5)
(383 10) (384 4) (386 4) (388 5) (391 6)
(392 10) (393 10) (394 12) (395 15) (396 3)
(399 3) (401 7) (402 6) (403 5) (416 6)
(417 5) (418 11) (423 6) (427 6) (431 7)
(432 13) (433 7) (434 6) (435 6) (438 11)
(442 5) (444 9) (445 11) (446 6) (448 8)
(456 5) (457 16) (458 12) (459 7) (460 7)
(461 10) (464 14) (471 4) (472 10) (473 10)
(475 5) (476 5) (477 4) (478 18) (480 6)
(481 7) (482 3) (483 16) (487 12) (488 4)
(491 17) (492 12) (494 8) (495 11) (496 4)
(497 4) (498 7) (500 8) (501 10) (502 9)
(504 8) (505 19) (510 8) (511 5) (512 6)
(514 4) (515 8) (517 13) (518 3) (520 8)
(521 16) (522 10) (523 4) (525 6) (526 5)
(527 6) (528 10) (532 7) (533 6) (535 7)
(536 8) (539 7) (546 6) (547 7) (549 3)
(550 5) (551 7) (553 6) (554 7) (555 10)
(556 3) (557 6) (559 4) (563 5) (566 4)
(567 7) (568 7) (573 6) (575 3) (576 3)
(581 5) (585 3) (593 3)

NAME:12C_1522.3_1313EC36_Methionine (2TMS)
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:152001-10-1
RI:1522
RT:8.924
NUM PEAKS: 108
(73 999) (78 21) (79 29) (93 23) (108 5)
(122 4) (128 997) (129 132) (166 10) (176 1000)
(177 142) (178 78) (182 7) (209 8) (225 7)
(226 9) (229 7) (238 8) (241 3) (249 5)
(250 53) (251 13) (252 7) (269 8) (270 6)
(288 6) (290 10) (293 55) (295 12) (297 5)
(298 8) (300 4) (303 3) (312 6) (313 10)
(314 4) (315 8) (317 4) (324 3) (345 8)
(354 7) (367 5) (368 8) (369 6) (370 4)
(371 8) (374 6) (379 5) (380 3) (381 9)
(382 6) (383 7) (386 4) (387 5) (388 9)
(389 4) (398 6) (400 3) (404 3) (405 3)
(406 7) (410 4) (419 5) (420 5) (421 9)
(423 3) (424 4) (426 6) (432 4) (433 7)
(434 7) (435 4) (439 5) (444 6) (452 8)
(457 6) (461 7) (462 10) (466 4) (467 6)
(472 5) (478 6) (479 5) (480 4) (484 7)
(485 7) (489 4) (491 4) (492 5) (493 4)
(496 4) (497 7) (500 7) (501 4) (509 5)
(513 5) (516 3) (517 4) (520 3) (524 4)
(526 6) (532 4) (544 5) (545 3) (548 10)
(555 5) (559 4) (560 4)

NAME:12C_1560.7_1191EC08_Cysteine (3TMS)
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:156002-10-1
RI:1561
RT:9.691
NUM PEAKS: 49

(72 25)	(73 1000)	(74 66)	(75 68)	(86 15)
(89 7)	(95 3)	(98 3)	(99 3)	(100 171)
(101 25)	(102 5)	(105 9)	(114 5)	(115 20)
(116 44)	(117 28)	(129 9)	(131 9)	(132 60)
(133 32)	(134 8)	(138 4)	(144 5)	(147 94)
(148 30)	(149 14)	(155 10)	(158 4)	(159 3)
(163 4)	(174 28)	(203 4)	(204 6)	(205 3)
(212 3)	(218 166)	(219 33)	(220 184)	(221 40)
(222 22)	(232 5)	(243 3)	(246 3)	(247 4)
(257 3)	(294 7)	(295 3)	(322 3)	

NAME:12C_1281.5_1313EC36_Ethanolamine (3TMS)
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer |RI:1282 |RI:1282
CASNO:128002-10-1
RI:1282
RT:6.152
SOURCE:C:\KOPKA\AMDIS32\LIB\File2.msp
NUM PEAKS: 25

(72 19)	(73 1000)	(74 79)	(75 133)	(86 276)
(87 20)	(88 19)	(100 284)	(101 33)	(102 25)
(103 26)	(114 30)	(117 30)	(130 53)	(131 45)
(133 83)	(134 8)	(144 24)	(148 14)	(158 7)
(172 10)	(174 945)	(175 165)	(176 57)	(188 8)

NAME:12C_1364.2_1313EC11_Uracil (2TMS)
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:136001-10-1
RI:1364
RT:7.160
NUM PEAKS: 30

(72 155)	(73 836)	(74 77)	(86 38)	(96 27)
(98 37)	(99 1000)	(100 270)	(101 91)	(103 22)
(105 25)	(109 39)	(113 231)	(114 21)	(117 37)
(126 260)	(127 37)	(131 109)	(133 50)	(147 605)
(148 91)	(153 26)	(169 32)	(239 24)	(241 624)
(242 130)	(243 43)	(255 318)	(256 270)	(257 64)

NAME:12C_1372.9_1313EC75_Fumaric acid (2TMS)
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:137001-10-1
RI:1373
RT:7.260
NUM PEAKS: 37

(72 44)	(73 1000)	(74 116)	(75 637)	(77 32)
(80 12)	(82 49)	(83 207)	(84 81)	(111 12)
(112 19)	(115 105)	(117 23)	(127 62)	(128 21)
(133 150)	(134 22)	(135 32)	(143 183)	(144 26)
(147 940)	(148 150)	(149 114)	(155 73)	(156 29)
(157 37)	(171 21)	(184 23)	(199 16)	(207 20)
(215 16)	(217 43)	(242 12)	(245 650)	(246 139)
(247 70)	(259 29)			

NAME:12C_1450.0_1313EC75_[690; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

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CASNO:144007-10-1
RI:1450
RT:8.1600
NUM PEAKS:  162
( 70    5) ( 71    5) ( 72   37) ( 73 1000) ( 74  118)
( 75  311) ( 76   37) ( 77   19) ( 81    2) ( 83    1)
( 84    3) ( 87   19) ( 89   20) ( 90    2) ( 91    3)
( 92    3) ( 93    1) ( 97    5) ( 98    3) (100   46)
(101   17) (102   17) (103   30) (104    8) (105   12)
(110    4) (114    7) (115   25) (116  110) (117  232)
(118   25) (119   26) (120    3) (122    1) (123    2)
(125    9) (128   15) (129    5) (130  164) (131   56)
(132   18) (133   43) (134    6) (135    4) (136    2)
(137    4) (143    1) (144   27) (146   12) (147  128)
(148   23) (149   26) (150    5) (151    6) (154   10)
(157   21) (158    6) (159   11) (160  270) (161   38)
(162    6) (163   43) (164    7) (165    3) (169    2)
(170    6) (172    8) (174    2) (175    9) (177    1)
(180    3) (185    1) (187    1) (188    4) (189    3)
(200    1) (201   10) (202    5) (204    1) (205    8)
(207    2) (211    6) (212    6) (215    7) (217    2)
(220    3) (221    1) (228    2) (232    7) (234    9)
(236    5) (245   19) (246    6) (247    5) (248    5)
(253    2) (254    3) (256    1) (257    2) (260    3)
(262    7) (264    3) (277    2) (278    6) (287    3)
(288    4) (290    2) (300    2) (301    5) (302    7)
(308    1) (319    1) (320    9) (321    3) (322    4)
(335    1) (336    2) (353    4) (354    4) (369    3)
(376    2) (387    3) (404    1) (407    1) (410    5)
(411    2) (415    3) (421    3) (422    5) (427    6)
(430    3) (435    3) (438    3) (441    2) (449    1)
(464    3) (467    3) (469    7) (470    4) (474    2)
(477    4) (484    1) (487    1) (494    4) (500    1)
(501    2) (503    2) (510    2) (511    1) (516    1)
(517    4) (519    2) (520    1) (522    6) (524    1)
(533    6) (536    1) (540    2) (541    3) (543    1)
(552    7) (564    1)

NAME:12C_1503.9_1313EC75_Erythritol (4TMS)
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:150002-10-1
RI:1504
RT:8.781
NUM PEAKS:  181
( 73 1000) ( 74   80) ( 75  187) ( 76   14) ( 87    6)
( 88    6) ( 89   68) ( 90    5) (101   43) (103  155)
(104   15) (105   11) (115   37) (116   51) (117  136)
(118   12) (119   13) (120    3) (122    2) (129   53)
(130    4) (131   38) (132    4) (133   87) (134   11)
(135   10) (143   28) (144    3) (145    9) (147  338)
(148   51) (149   35) (150    4) (151    3) (157   10)
(158    3) (161    5) (162    2) (163   14) (164    3)
(171    7) (173    6) (174    3) (175   10) (177    5)
(178    2) (185    4) (187    5) (188    2) (189   56)
(190   11) (191   40) (192    8) (193    3) (195    2)
(198    2) (199    4) (201   21) (202    3) (203   13)
(204   53) (205   90) (206   19) (207    9) (209    5)
(215    7) (216    3) (217  173) (218   35) (219   13)
(221    9) (222    5) (229    6) (230    3) (231   11)
(233    2) (238    3) (240    2) (244    2) (247    5)
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(248	4)	(249	3)	(251	2)	(259	5)	(260	3)
(263	1)	(264	2)	(265	2)	(266	2)	(274	2)
(275	19)	(276	6)	(277	8)	(278	3)	(279	2)
(280	3)	(281	2)	(285	2)	(286	3)	(287	2)
(288	2)	(289	3)	(290	3)	(291	8)	(292	3)
(293	14)	(294	5)	(305	4)	(306	3)	(307	13)
(308	4)	(311	2)	(312	3)	(316	2)	(319	7)
(320	6)	(321	3)	(322	2)	(325	2)	(326	3)
(327	2)	(328	3)	(334	2)	(335	2)	(336	3)
(337	2)	(342	2)	(347	2)	(349	2)	(353	4)
(361	2)	(372	2)	(373	2)	(374	3)	(376	2)
(382	2)	(391	3)	(400	2)	(409	3)	(415	1)
(419	2)	(420	2)	(424	2)	(428	3)	(429	2)
(433	2)	(435	2)	(440	2)	(442	3)	(447	2)
(454	2)	(455	2)	(456	2)	(457	2)	(458	2)
(459	1)	(462	2)	(463	3)	(476	1)	(478	2)
(482	2)	(484	2)	(492	2)	(493	2)	(495	2)
(501	2)	(506	3)	(507	3)	(516	3)	(522	2)
(523	2)	(529	2)	(532	3)	(537	2)	(539	2)
(540	2)	(544	2)	(552	1)	(564	2)	(571	2)
(575	2)								

NAME:12C_1694.8_1313EC75_[746; Ribonic acid-1,4-lactone (3TMS)]
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:169001-10-1
RI:1695
RT:10.265
NUM PEAKS: 27

(73	1000)	(74	77)	(75	69)	(101	36)	(102	70)
(117	211)	(130	64)	(133	105)	(139	7)	(143	14)
(147	260)	(148	31)	(149	56)	(153	6)	(189	23)
(191	21)	(203	14)	(215	54)	(217	23)	(231	32)
(246	25)	(248	16)	(259	33)	(349	16)	(355	7)
(413	11)	(564	11)						

NAME:12C_1670.8_1313EC75_Arabinose methoxyamine (4TMS)
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer \|RI:1671 \|RI:1671 \|RI:1671
CASNO:167002-10-1
RI:1671
RT:10.078
SOURCE:C:\KOPKA\AMDIS32\LIB\File2.msp
NUM PEAKS: 142

(70	8)	(71	6)	(72	22)	(73	1000)	(74	88)
(75	83)	(76	4)	(82	3)	(83	3)	(84	4)
(85	7)	(86	6)	(87	8)	(88	5)	(89	56)
(90	5)	(96	1)	(99	6)	(100	27)	(101	23)
(102	10)	(103	397)	(104	37)	(105	31)	(111	2)
(112	2)	(113	5)	(114	8)	(115	9)	(116	8)
(117	43)	(118	4)	(119	8)	(125	1)	(126	2)
(127	3)	(128	4)	(129	52)	(130	11)	(131	35)
(132	5)	(133	68)	(134	8)	(136	1)	(140	2)
(141	1)	(142	5)	(143	14)	(144	3)	(145	7)
(146	1)	(147	200)	(148	31)	(149	21)	(150	2)
(151	1)	(152	1)	(154	1)	(156	1)	(157	3)
(158	5)	(159	3)	(160	40)	(161	10)	(162	2)
(163	8)	(164	1)	(165	1)	(168	9)	(169	2)
(170	4)	(171	1)	(172	6)	(173	5)	(174	7)
(175	6)	(176	1)	(177	3)	(184	1)	(186	1)
(187	1)	(188	1)	(189	44)	(190	15)	(191	16)
(192	3)	(193	1)	(198	3)	(199	1)	(200	2)

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(201    3) (203    3) (204   18) (205   21) (206    4)
(207    3) (216    5) (217  199) (218   41) (219   18)
(220    2) (221    5) (222    1) (223    1) (228    1)
(230    1) (231    3) (232    2) (233   15) (234    6)
(235    1) (240    1) (242    3) (243    1) (244    1)
(248    2) (250    1) (256    3) (257    2) (258    5)
(259    1) (260    1) (262    5) (263    1) (272    1)
(274    2) (276    1) (277   15) (278    5) (279    2)
(291    3) (292    1) (306    3) (307   65) (308   19)
(309    9) (310    1) (330    1) (331    1) (332    1)
(361    1) (362    1)

NAME:12C_1726.7_1313EC36_Fucose methoxyamine (4TMS)
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:173002-10-1
RI:1727
RT:10.513
NUM PEAKS:  58
( 72   15) ( 73 1000) ( 74   73) ( 75  131) ( 83   25)
(101   11) (103   84) (104   13) (105  105) (106   11)
(115   16) (117  495) (118   44) (119   15) (131   35)
(133   70) (147  257) (148   47) (149   35) (157   19)
(158   12) (174   29) (176    7) (187   14) (190   23)
(191   19) (203   14) (204   13) (205   30) (209   11)
(211    8) (217   99) (218   12) (231   12) (242    6)
(245   39) (246   71) (247   11) (255    7) (263    6)
(267    7) (268   11) (276    7) (299    7) (318    8)
(319   19) (320   13) (321    7) (378   11) (380    9)
(407    8) (410    7) (437    7) (444   10) (493    7)
(504    8) (519    8) (555    6)

NAME:12C_1784.9_1313EC75_[798; Ribonic acid (5TMS)]
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:179001-10-1
RI:1785
RT:10.966
NUM PEAKS:  44
( 72   16) ( 73 1000) ( 74   81) ( 75   50) ( 89   17)
(101   13) (102   19) (103  207) (104   18) (105    8)
(117   50) (119    6) (130   17) (131   26) (132    6)
(133   76) (134    8) (143   28) (145    4) (147  282)
(148   38) (175    5) (189   38) (190    7) (191   16)
(205   33) (206    6) (207    7) (217  134) (218   24)
(219   16) (221   15) (222    5) (257    7) (277   15)
(278    6) (292  128) (293   38) (294   16) (305   19)
(306    7) (307   18) (331    7) (333   15)

NAME:12C_1806.2_1313EC75_[549; 2-Keto-D-gluconic acid (5TMS)]
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:181004-10-1
RI:1806
RT:11.131
NUM PEAKS:  57
( 73 1000) ( 74   98) ( 90    8) (102   16) (128   11)
(131   24) (133   40) (134   12) (147  160) (159   17)
(161   12) (162   12) (187  131) (188   28) (213   15)
(215   18) (217  126) (218   33) (219   23) (245    8)
(246   10) (254    9) (257   56) (265    6) (266   11)
(268    8) (280    9) (285    9) (302    9) (303   14)
(304    8) (313   11) (327   12) (352   11) (363   11)
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(365   13) (369    8) (399   11) (400    8) (401    9)
(410    7) (437   37) (441   10) (475   11) (488   13)
(494   14) (498   11) (499   14) (510   10) (522   10)
(528   15) (536   15) (555    8) (563    8) (573    4)
(593    2) (599    2)

NAME:12C_1842.1_1313EC75_[693; 2-Furan-2-hydroxyacetic acid (2TMS)]
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:184002-10-1
RI:1842
RT:11.411
NUM PEAKS:  122
( 70    8) ( 71    7) ( 72   21) ( 73 1000) ( 74   90)
( 75  144) ( 76   10) ( 77   12) ( 78    1) ( 79    4)
( 80   12) ( 81   83) ( 82    6) ( 83    7) ( 85   11)
( 87    5) ( 88    4) ( 89   13) ( 92    2) ( 93   11)
( 94    7) ( 95   46) ( 96   11) ( 97   14) ( 98   19)
( 99   11) (100    5) (101   41) (106    2) (107    8)
(108    2) (109    4) (110    3) (111    4) (112   11)
(113    3) (115    6) (117   96) (118    7) (119   15)
(121    5) (122    1) (123    6) (124    4) (125   12)
(126    7) (127    8) (131   23) (132    5) (133   65)
(134   10) (135    7) (137    5) (138   23) (139   13)
(140    7) (147  191) (148   28) (149   19) (150    2)
(151    7) (152    4) (153   49) (154   49) (155   19)
(166   23) (167   55) (168   11) (169  860) (170  497)
(171   86) (172   14) (175    5) (179    8) (180    1)
(181    5) (182    8) (183    4) (193    2) (194   10)
(195   23) (196    3) (197    2) (199    2) (205   18)
(206    3) (207    2) (209    1) (210   10) (211    3)
(212    3) (227    2) (239   10) (240    3) (241   28)
(242   43) (243   14) (255    5) (256    2) (257    2)
(267    1) (268    2) (269   17) (270    6) (271    4)
(283    3) (284   26) (285    4) (286    2) (313    1)
(329   12) (330    4) (331    2) (358    2) (359   13)
(360    3) (373    1) (374   20) (375    7) (376    4)
(377    1) (390    1)

NAME:12C_1848.6_1313EC75_[708; Glucose methoxyamine (5TMS)]
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:185003-10-1
RI:1849
RT:11.461
NUM PEAKS:  137
( 70    4) ( 71    6) ( 72   18) ( 73 1000) ( 74   86)
( 75  120) ( 76    7) ( 77    6) ( 82   10) ( 83    4)
( 84    2) ( 85    8) ( 86    4) ( 87    6) ( 88    4)
( 89   83) ( 90    7) ( 91    4) ( 92    1) ( 94    1)
( 99    5) (100   16) (101   20) (102    8) (103  195)
(104   20) (105   19) (106    3) (111    4) (112    2)
(113    4) (114    4) (115    8) (117   71) (118    6)
(119    9) (120    1) (126    3) (127    5) (129  104)
(130   44) (131   23) (133   65) (134    8) (135    6)
(141    2) (142    7) (143   13) (144    2) (145    9)
(146    2) (147  109) (148   18) (149   21) (150    3)
(151    2) (152    1) (157  195) (158   29) (159   13)
(160   47) (161   44) (162    7) (163   48) (164    8)
(165    4) (168    1) (172    4) (174    6) (175    4)
(176    1) (177    5) (178    1) (180    2) (182    1)
(186    2) (187    2) (188    2) (189   77) (190   15)
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(191 14) (192 2) (193 1) (196 1) (198 1)
(200 1) (202 1) (203 7) (204 11) (205 49)
(206 10) (212 1) (214 5) (215 3) (216 3)
(217 47) (218 16) (219 15) (220 3) (228 2)
(229 11) (230 5) (231 9) (232 4) (233 10)
(234 2) (235 7) (236 1) (237 1) (240 1)
(243 4) (244 50) (245 13) (246 7) (247 30)
(248 7) (249 3) (259 3) (260 1) (261 1)
(262 1) (268 1) (270 2) (274 1) (275 1)
(276 1) (278 1) (291 1) (302 2) (304 2)
(305 1) (319 27) (320 9) (321 4) (322 1)
(333 1) (337 1)

NAME:12C_2113.2_1313EC36_[697; Ribose-5-phosphate methoxyamine (5TMS)]
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:211003-10-1
RI:2113
RT:13.210
NUM PEAKS: 16
(73 1000) (74 94) (89 45) (129 96) (133 74)
(147 155) (157 20) (207 19) (211 57) (217 123)
(299 117) (300 41) (315 157) (316 50) (317 31)
(459 18)

NAME:12C_2225.2_1313EC36_Octadecenoic acid (1TMS)
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:223003-10-1
RI:2225
RT:13.896
NUM PEAKS: 126
(70 45) (71 28) (72 42) (73 1000) (75 767)
(76 50) (77 44) (80 13) (81 109) (82 71)
(83 95) (84 111) (85 25) (86 17) (88 12)
(89 20) (94 22) (95 93) (96 137) (97 82)
(98 100) (99 27) (100 47) (101 29) (102 26)
(107 11) (108 14) (109 47) (110 50) (111 31)
(112 22) (113 12) (114 8) (116 57) (117 394)
(118 37) (119 33) (121 14) (122 11) (123 37)
(124 28) (125 16) (126 7) (128 9) (129 376)
(130 65) (131 77) (132 115) (137 14) (138 20)
(139 11) (143 22) (144 10) (145 146) (146 21)
(149 12) (151 7) (152 23) (153 6) (155 11)
(158 12) (159 15) (162 6) (166 17) (170 15)
(171 19) (172 14) (173 15) (180 23) (183 11)
(184 9) (185 39) (186 18) (187 10) (188 12)
(190 12) (199 35) (200 28) (208 7) (210 4)
(214 7) (218 26) (220 13) (222 23) (235 8)
(240 6) (248 8) (264 21) (268 4) (272 5)
(274 7) (275 8) (283 5) (303 8) (309 6)
(337 10) (338 8) (339 75) (340 28) (354 8)
(362 7) (363 7) (378 4) (385 5) (407 11)
(412 8) (413 7) (446 6) (449 8) (454 4)
(456 6) (459 4) (471 6) (472 10) (475 11)
(480 9) (486 4) (487 5) (513 6) (520 5)
(521 7) (527 5) (550 4) (568 6) (586 4)
(588 4)

NAME:12C_3270.3_1313EC36_Ergosterol (1TMS)
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:327001-10-1

RI:3270
RT:19.000
NUM PEAKS: 189
(70 153) (71 80) (72 19) (73 1000) (74 107)
(75 502) (76 64) (77 163) (78 39) (79 251)
(80 30) (81 452) (82 78) (83 274) (84 26)
(85 27) (86 10) (87 18) (88 9) (89 43)
(90 11) (91 309) (92 39) (93 193) (94 32)
(95 188) (96 24) (97 81) (98 15) (99 12)
(101 30) (102 19) (103 43) (104 19) (105 224)
(106 27) (107 133) (108 21) (109 130) (110 16)
(111 33) (113 10) (114 4) (115 190) (116 50)
(117 140) (118 44) (119 323) (120 38) (121 55)
(122 8) (123 47) (124 9) (125 88) (126 18)
(127 57) (128 242) (129 373) (130 87) (131 429)
(132 69) (133 92) (134 14) (135 42) (136 8)
(137 28) (138 5) (139 17) (140 6) (141 222)
(142 142) (143 453) (144 272) (145 294) (146 57)
(147 74) (148 11) (149 27) (150 9) (151 22)
(152 55) (153 88) (154 60) (155 217) (156 88)
(157 392) (158 128) (159 234) (160 41) (161 19)
(162 5) (163 21) (164 11) (165 89) (166 43)
(167 80) (168 64) (169 224) (170 80) (171 165)
(172 41) (173 43) (174 9) (175 10) (176 6)
(177 8) (178 26) (179 40) (180 24) (181 85)
(182 60) (183 169) (184 53) (185 129) (186 31)
(187 18) (188 4) (189 9) (191 11) (192 7)
(193 22) (194 25) (196 51) (197 165) (198 57)
(199 111) (200 23) (201 22) (202 7) (205 10)
(206 5) (207 13) (208 8) (209 58) (211 228)
(212 60) (213 83) (214 16) (215 7) (219 7)
(223 39) (224 19) (225 49) (226 53) (227 43)
(228 9) (229 5) (238 29) (239 55) (240 14)
(241 6) (247 3) (248 3) (251 68) (252 33)
(253 164) (254 37) (255 6) (265 21) (266 7)
(267 13) (268 4) (279 12) (280 12) (281 8)
(293 13) (294 6) (295 4) (310 5) (323 5)
(326 10) (327 6) (335 6) (336 17) (337 227)
(338 82) (339 18) (343 6) (363 317) (364 119)
(365 21) (377 14) (378 79) (379 31) (380 5)
(467 9) (468 53) (469 28) (470 8)

NAME:12C_1580.7_1313EC75_[829; 1-Phenylethanol (1TMS)]
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:158002-10-1
RI:1581
RT:9.378
NUM PEAKS: 10
(82 34) (179 1000) (180 165) (181 44) (193 105)
(194 19) (267 71) (268 15) (269 6) (284 6)

NAME:12C_2109.7_1313EC75_[662; Ribose-5-phosphate methoxyamine (BP) (5TMS)]
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:211004-10-1
RI:2110
RT:13.188
NUM PEAKS: 47
(72 27) (73 1000) (74 90) (75 151) (77 24)
(89 42) (98 13) (100 40) (101 45) (104 8)
(105 22) (114 12) (115 15) (117 75) (119 14)

(129 122) (130 31) (131 42) (132 33) (133 69)
(135 24) (138 7) (143 14) (145 21) (147 232)
(158 31) (160 40) (175 5) (189 17) (191 16)
(195 10) (207 13) (211 46) (212 13) (217 118)
(218 29) (219 10) (225 13) (299 96) (300 31)
(301 13) (315 143) (316 39) (321 8) (357 16)
(387 9) (403 14)

NAME:12C_2125.3_1313EC75_[832; Dopamine (4TMS)]
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:213003-10-1
RI:2125
RT:13.287
NUM PEAKS: 53
(72 18) (73 816) (74 58) (75 62) (77 7)
(86 118) (89 9) (96 5) (100 38) (102 20)
(103 20) (104 14) (114 9) (115 9) (117 58)
(128 12) (130 23) (131 27) (133 29) (139 7)
(143 13) (147 282) (148 40) (161 8) (172 13)
(174 1000) (175 190) (176 68) (177 6) (178 7)
(188 8) (189 19) (204 17) (205 21) (207 5)
(216 7) (217 26) (218 9) (248 4) (259 9)
(288 5) (290 17) (291 12) (299 6) (304 9)
(307 10) (344 5) (355 5) (396 6) (443 5)
(475 4) (591 4) (599 3)

NAME:12C_2155.6_1313EC75_[795; Erythritol (4TMS)]
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:216003-10-1
RI:2156
RT:13.479
NUM PEAKS: 106
(72 14) (73 1000) (74 86) (80 5) (84 7)
(86 10) (88 22) (93 3) (94 3) (100 6)
(103 163) (104 18) (105 12) (107 4) (108 3)
(114 7) (116 19) (117 86) (118 9) (119 7)
(127 5) (128 7) (129 46) (130 17) (131 16)
(132 4) (133 46) (134 7) (135 5) (140 4)
(141 6) (142 26) (143 15) (144 12) (145 3)
(146 26) (147 239) (148 36) (149 27) (150 3)
(151 3) (155 4) (157 27) (158 14) (163 3)
(168 9) (169 9) (172 7) (173 16) (174 43)
(175 7) (179 3) (180 4) (181 3) (184 3)
(189 20) (191 12) (196 3) (197 14) (198 7)
(200 11) (201 4) (202 3) (203 5) (204 17)
(205 60) (206 14) (207 9) (216 4) (217 77)
(218 19) (219 6) (221 12) (228 4) (229 25)
(230 6) (231 3) (232 4) (243 9) (256 7)
(257 7) (259 3) (269 4) (311 5) (313 4)
(314 11) (315 7) (319 8) (320 3) (339 6)
(343 4) (344 5) (345 26) (346 9) (347 4)
(357 6) (370 5) (371 4) (375 5) (429 6)
(433 3) (435 3) (519 10) (520 3) (521 3)
(523 3)

NAME:12C_2162.3_1313EC75_[648; Ethylamine (2TMS)]
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:216002-10-1
RI:2162
RT:13.521

NUM PEAKS: 54
(72 18) (73 1000) (74 79) (75 51) (86 127)
(87 17) (89 31) (100 88) (101 23) (102 17)
(103 161) (104 15) (106 4) (115 7) (117 64)
(118 9) (129 34) (130 20) (132 6) (133 39)
(134 6) (143 9) (157 10) (172 25) (173 9)
(174 283) (175 54) (176 20) (185 12) (189 17)
(190 8) (199 5) (200 4) (204 13) (205 45)
(206 10) (207 5) (216 10) (217 93) (218 19)
(219 9) (231 4) (241 16) (259 6) (267 7)
(272 16) (287 15) (288 6) (305 7) (306 3)
(307 15) (314 11) (315 12) (346 5)

NAME:12C_2168.9_1313EC75_[705; 2-Ketogluconic acid (5TMS)]
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:217002-10-1
RI:2169
RT:13.563
NUM PEAKS: 52
(72 21) (73 1000) (74 81) (75 70) (79 5)
(86 63) (87 12) (89 11) (100 35) (102 10)
(103 35) (115 6) (116 5) (117 26) (129 37)
(130 16) (131 28) (133 34) (134 9) (141 30)
(142 8) (145 4) (147 269) (148 43) (149 25)
(150 5) (156 5) (157 17) (167 4) (170 4)
(172 8) (174 104) (175 22) (176 8) (189 16)
(191 41) (192 8) (205 17) (207 7) (215 11)
(217 47) (218 13) (257 45) (258 12) (303 12)
(304 7) (319 12) (425 3) (436 9) (437 40)
(438 20) (439 9)

NAME:12C_2180.5_1313EC75_[733; Threitol (4TMS)]
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:218001-10-1
RI:2181
RT:13.637
NUM PEAKS: 128
(70 7) (72 20) (73 1000) (74 89) (75 131)
(76 9) (77 6) (80 8) (81 7) (82 7)
(83 25) (86 11) (87 7) (88 6) (89 43)
(94 4) (95 14) (97 4) (98 5) (100 11)
(101 17) (102 8) (103 194) (104 18) (105 11)
(107 7) (109 5) (114 9) (115 7) (116 20)
(117 74) (119 8) (125 3) (127 5) (128 9)
(129 40) (130 15) (131 22) (132 5) (133 51)
(134 6) (139 5) (140 4) (142 32) (144 20)
(145 7) (146 43) (147 222) (148 35) (149 25)
(150 4) (152 4) (155 5) (156 5) (157 14)
(158 29) (159 6) (160 8) (163 5) (167 5)
(168 8) (169 9) (172 10) (173 24) (174 66)
(175 12) (176 4) (181 7) (183 5) (185 10)
(186 9) (187 5) (188 3) (189 18) (190 5)
(191 10) (195 3) (197 26) (198 8) (199 3)
(200 6) (202 3) (203 3) (205 38) (206 8)
(207 6) (215 4) (216 6) (217 81) (218 20)
(219 8) (221 9) (223 6) (229 14) (230 4)
(232 6) (243 8) (253 4) (255 4) (256 7)
(268 5) (270 3) (271 4) (277 4) (287 5)
(291 3) (295 4) (307 5) (313 5) (314 12)
(315 7) (339 7) (340 3) (343 5) (344 5)

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(345   40) (346   12) (347    4) (370    5) (371    3)
(375    6) (429    6) (430    3) (433    4) (518    3)
(519    8) (523    8) (524    4)

NAME:12C_2245.5_1313EC75_Octadecanoic acid (1TMS)
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:225002-10-1
RI:2246
RT:14.001
NUM PEAKS:  124
( 70   33) ( 71   65) ( 72   50) ( 73  932) ( 74  104)
( 75 1000) ( 76   73) ( 77   57) ( 78    3) ( 79   29)
( 80    4) ( 81   78) ( 82   12) ( 83   87) ( 84   26)
( 85   39) ( 86   13) ( 88    7) ( 89   29) ( 90    5)
( 91   13) ( 92    3) ( 93   27) ( 94    4) ( 95   69)
( 96   12) ( 97   66) ( 98   48) ( 99   28) (100    4)
(101   15) (102    6) (105   28) (106    3) (107   14)
(109   22) (110    4) (111   32) (112   14) (113    6)
(115   10) (116   65) (117  947) (118   94) (119   39)
(121   11) (123    7) (125    9) (126    4) (127    6)
(128    4) (129  493) (130   64) (131  162) (132  487)
(133  105) (134   25) (135   12) (137    3) (139    5)
(140    4) (141    5) (143   51) (144    7) (145  282)
(146   39) (149    5) (151    3) (153    5) (154    9)
(155    7) (157   15) (158    3) (159   33) (160    6)
(163    3) (167    4) (168    3) (171   28) (172    4)
(173    8) (174    4) (185   44) (186    7) (187   25)
(188    9) (199   12) (201   76) (202   13) (203    4)
(210    3) (213   10) (214    3) (215   11) (216    3)
(223    5) (227   13) (228    3) (229    6) (230    3)
(241   13) (242    3) (243   11) (244    3) (255    7)
(257   17) (258    4) (269    3) (271    7) (283    3)
(285    3) (297   15) (298    6) (299    6) (313   15)
(314    5) (340   19) (341  216) (342   68) (343   17)
(355    3) (356   37) (357   12) (358    3)

NAME:12C_2328.1_1313EC75_Glucose-6-phosphate methoxyamine (6TMS)
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:233002-10-1
RI:2328
RT:14.440
NUM PEAKS:  123
( 70    4) ( 72   17) ( 73 1000) ( 74   88) ( 75   83)
( 76    4) ( 77   10) ( 82    7) ( 86    6) ( 87    6)
( 88    3) ( 89   34) ( 90    3) ( 99    5) (100   12)
(101   38) (102   11) (104    4) (105   24) (106    4)
(107    3) (113    6) (114   10) (115   12) (116   16)
(119    7) (121    3) (127    4) (129   69) (130   17)
(131   27) (132    4) (133   65) (134    9) (135   16)
(137    6) (138    3) (141    3) (142    5) (143   11)
(145    7) (147  141) (148   22) (149   18) (150    3)
(151    7) (156    3) (157   35) (158    9) (159    4)
(160   94) (161   19) (162    4) (163    6) (169    4)
(173    4) (181    8) (189   11) (190    3) (191   16)
(193   10) (195    8) (196    3) (197    3) (204   17)
(205    7) (207   16) (208    4) (209    3) (210    4)
(211   43) (212    9) (213    5) (215    4) (216    6)
(217   36) (218    9) (219    4) (221    3) (225   13)
(226    3) (227    9) (228    6) (229    5) (231    7)
(243    5) (244    3) (246    3) (253    4) (268    3)
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(269 5) (274 3) (283 4) (285 5) (298 10)
(299 104) (300 30) (301 14) (302 3) (313 3)
(314 7) (315 41) (316 12) (317 6) (331 13)
(332 4) (341 6) (342 3) (356 6) (357 37)
(358 12) (359 6) (373 3) (385 3) (386 30)
(387 122) (388 47) (389 25) (390 7) (470 4)
(471 12) (472 6) (473 3)

NAME:12C_2383.7_1313EC75_[724; Glycerol (3TMS)]
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:238002-10-1
RI:2384
RT:14.735
NUM PEAKS: 34
(72 16) (73 1000) (74 80) (75 108) (87 7)
(89 36) (103 153) (104 11) (116 8) (117 196)
(118 17) (129 29) (130 9) (131 17) (133 41)
(142 35) (143 11) (144 15) (147 208) (148 30)
(149 21) (158 89) (159 23) (160 19) (171 7)
(173 9) (183 15) (189 13) (201 8) (205 34)
(216 8) (217 71) (218 18) (276 12)

NAME:12C_2564.4_1313EC75_[945; Galactofuranose-6-phosphate (7TMS)]
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:256001-10-1
RI:2564
RT:15.695
NUM PEAKS: 263
(72 20) (73 1000) (74 85) (75 90) (76 14)
(77 12) (79 12) (84 17) (86 5) (87 6)
(88 8) (89 47) (90 6) (91 7) (92 3)
(96 5) (98 3) (100 9) (101 31) (103 102)
(105 16) (106 9) (107 6) (115 12) (116 18)
(117 28) (119 11) (120 5) (121 7) (128 7)
(129 76) (130 17) (131 34) (132 8) (133 80)
(134 15) (135 19) (136 3) (137 10) (139 3)
(142 10) (143 10) (144 9) (145 9) (146 6)
(147 160) (148 24) (151 5) (153 5) (156 8)
(157 35) (158 10) (159 8) (162 7) (163 12)
(165 3) (166 3) (171 4) (172 13) (173 17)
(174 8) (175 8) (176 4) (181 9) (185 5)
(186 6) (188 7) (189 14) (190 5) (191 17)
(195 8) (196 6) (197 3) (200 7) (201 7)
(202 8) (203 10) (204 16) (205 14) (206 6)
(207 15) (208 6) (210 5) (211 34) (212 5)
(214 7) (216 7) (217 50) (218 14) (219 4)
(220 6) (222 5) (223 3) (225 15) (226 8)
(227 10) (228 7) (229 5) (230 5) (231 6)
(232 6) (233 6) (235 6) (236 4) (239 3)
(240 4) (241 4) (245 5) (249 7) (250 4)
(251 6) (253 4) (259 6) (260 5) (264 4)
(265 6) (266 4) (267 8) (268 4) (269 9)
(270 7) (271 4) (273 6) (274 6) (275 5)
(276 6) (281 5) (282 5) (283 10) (284 8)
(285 8) (291 3) (292 5) (293 4) (295 3)
(296 5) (298 10) (299 92) (300 25) (301 17)
(302 4) (303 3) (305 7) (306 5) (307 8)
(308 4) (312 3) (313 7) (314 5) (315 38)
(316 15) (317 9) (318 5) (319 5) (320 4)
(321 6) (324 4) (326 4) (327 5) (328 5)

(331 12) (332 9) (333 7) (340 5) (341 8)
(344 3) (346 3) (348 4) (349 6) (350 7)
(353 5) (354 3) (355 6) (356 10) (357 35)
(358 14) (359 8) (362 5) (363 4) (364 3)
(365 4) (369 6) (370 6) (371 7) (372 6)
(373 6) (377 4) (382 3) (384 4) (385 7)
(386 28) (387 115) (388 44) (389 28) (390 9)
(391 5) (393 3) (396 5) (400 4) (403 6)
(404 3) (405 6) (408 5) (409 4) (413 3)
(417 7) (418 6) (423 5) (427 4) (428 3)
(442 6) (443 3) (444 3) (448 7) (449 4)
(452 3) (457 6) (458 8) (459 3) (461 5)
(471 17) (472 7) (473 6) (475 3) (483 6)
(484 3) (485 3) (486 5) (487 6) (488 4)
(490 4) (491 4) (492 4) (495 7) (496 5)
(499 3) (500 4) (502 3) (509 5) (513 7)
(514 3) (517 6) (520 6) (525 4) (526 4)
(527 5) (528 4) (530 7) (531 6) (533 3)
(538 5) (541 3) (545 3) (547 4) (548 3)
(549 3) (550 3) (554 4) (560 4) (561 4)
(564 4) (566 4) (572 4)

NAME:12C_2619.2_1313EC75_[892; Sucrose (8TMS); alpha-D-Glc-(1,2)-beta-D-Fru]
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:262001-10-1
RI:2619
RT:15.985
NUM PEAKS: 126
(70 4) (71 6) (72 15) (73 1000) (74 87)
(75 134) (76 8) (77 10) (81 25) (83 5)
(85 9) (87 7) (88 3) (89 17) (91 3)
(95 3) (97 7) (99 9) (101 27) (102 5)
(103 193) (104 18) (105 11) (109 13) (111 10)
(113 10) (115 9) (116 18) (117 78) (118 8)
(119 8) (127 7) (129 177) (130 22) (131 39)
(132 10) (133 53) (134 7) (135 6) (139 4)
(141 6) (142 6) (143 28) (144 5) (145 18)
(146 3) (147 214) (148 34) (149 36) (150 5)
(151 4) (153 7) (155 46) (156 8) (157 37)
(158 6) (159 9) (161 3) (163 6) (169 89)
(170 15) (171 18) (172 3) (173 14) (175 5)
(177 6) (183 19) (184 3) (185 3) (189 33)
(190 8) (191 123) (192 22) (193 11) (199 25)
(200 4) (201 4) (203 13) (204 57) (205 23)
(206 7) (207 5) (215 6) (216 5) (217 307)
(218 74) (219 39) (220 6) (221 9) (227 3)
(229 6) (230 6) (231 15) (232 5) (233 7)
(234 3) (241 3) (242 4) (243 40) (244 11)
(245 13) (246 3) (247 6) (257 5) (259 20)
(260 6) (263 6) (271 27) (272 7) (273 11)
(274 3) (289 25) (290 7) (291 7) (305 5)
(319 9) (320 4) (331 20) (332 16) (333 7)
(360 13) (361 126) (362 45) (363 21) (364 5)
(377 4)

NAME:12C_2656.9_1313EC75_[559; Erythritol (4TMS)]
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:266001-10-1
RI:2657

RT:16.186
NUM PEAKS: 42
(70 175) (72 21) (73 1000) (74 83) (75 109)
(80 19) (81 16) (82 45) (83 15) (89 44)
(98 52) (99 122) (100 21) (103 162) (113 15)
(116 16) (117 56) (125 36) (127 130) (128 21)
(129 58) (131 29) (133 55) (147 201) (148 37)
(149 29) (155 15) (156 16) (169 37) (170 18)
(171 44) (185 29) (189 14) (196 25) (217 97)
(218 25) (238 14) (267 27) (268 44) (292 50)
(298 48) (323 21)

NAME:12C_2733.0_1313EC75_[840; Maltose methoxyamine (8TMS); alpha-D-Glc-(1,4)-D-Glc]
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:273002-10-1
RI:2733
RT:16.590
NUM PEAKS: 78
(70 3) (72 11) (73 1000) (74 85) (82 17)
(83 4) (85 5) (86 5) (87 4) (88 4)
(89 48) (90 3) (100 7) (101 19) (102 5)
(103 113) (104 9) (105 32) (106 3) (113 5)
(114 6) (115 5) (116 8) (117 77) (118 9)
(119 5) (128 4) (130 10) (131 14) (132 3)
(133 44) (140 3) (141 4) (143 15) (147 303)
(148 48) (149 26) (156 4) (160 85) (161 20)
(162 5) (163 5) (169 37) (170 7) (175 3)
(186 10) (187 3) (189 23) (190 3) (203 6)
(204 267) (205 112) (206 33) (207 11) (215 4)
(216 6) (218 17) (221 5) (222 3) (229 7)
(230 3) (243 19) (244 35) (245 12) (269 5)
(270 3) (271 18) (272 4) (307 6) (318 4)
(319 23) (320 9) (360 20) (361 169) (362 60)
(363 26) (390 3) (451 4)

NAME:12C_2826.4_1313EC75_[855; Squalene]
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:283001-10-1
RI:2826
RT:17.062
NUM PEAKS: 34
(70 112) (79 130) (80 53) (81 1000) (82 107)
(87 13) (92 36) (93 202) (95 280) (97 45)
(107 124) (108 40) (109 123) (118 14) (120 20)
(121 171) (122 37) (123 102) (132 9) (135 89)
(136 134) (137 123) (138 11) (149 107) (158 24)
(163 31) (173 24) (174 16) (175 26) (203 30)
(231 33) (259 18) (260 15) (363 10)

NAME:12C_2871.8_1313EC75_Isomaltose methoxyamine (8TMS); alpha-D-Glc-(1,6)-D-Glc (8TMS)
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:287001-10-1
RI:2872
RT:17.263
NUM PEAKS: 126
(70 5) (71 5) (72 15) (73 1000) (74 87)
(75 96) (81 15) (82 4) (83 4) (85 8)
(86 4) (87 7) (88 3) (89 33) (90 3)

(97 5) (99 8) (100 17) (101 36) (102 12)
(103 125) (104 12) (105 24) (109 7) (111 6)
(113 7) (114 6) (115 9) (116 20) (117 72)
(118 7) (119 6) (127 5) (128 4) (129 122)
(130 20) (131 30) (132 6) (133 56) (134 7)
(135 5) (139 3) (141 5) (142 7) (143 23)
(144 4) (145 9) (147 236) (148 37) (149 28)
(150 3) (151 3) (153 4) (155 18) (156 4)
(158 6) (159 5) (160 95) (161 39) (162 7)
(163 9) (169 67) (170 11) (171 8) (172 3)
(173 6) (174 3) (175 4) (177 4) (183 5)
(189 32) (190 9) (191 52) (192 9) (193 4)
(201 3) (203 14) (204 215) (205 57) (206 20)
(207 7) (215 5) (216 7) (217 135) (218 34)
(219 15) (221 9) (228 5) (229 7) (230 5)
(231 16) (232 5) (233 8) (234 3) (241 3)
(243 31) (244 10) (245 8) (246 5) (247 5)
(257 3) (259 6) (262 3) (271 24) (272 6)
(273 6) (274 4) (275 3) (291 7) (300 3)
(305 8) (306 4) (307 5) (317 3) (318 3)
(319 15) (320 5) (331 6) (332 5) (360 18)
(361 158) (362 56) (363 25) (364 9) (390 4)
(480 4)

NAME:12C_2906.7_1313EC75_Isomaltose methoxyamine (BP) (8TMS); alpha-D-Glc-(1,6)-D-Glc (8TMS)
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:291002-10-1
RI:2907
RT:17.418
NUM PEAKS: 64
(72 14) (73 1000) (74 80) (75 86) (81 13)
(87 7) (89 41) (100 18) (101 36) (102 11)
(103 166) (104 15) (105 15) (115 7) (117 69)
(118 8) (129 110) (130 17) (131 29) (132 6)
(133 73) (134 9) (143 20) (147 235) (148 37)
(149 28) (155 17) (157 19) (160 77) (161 41)
(163 9) (169 65) (170 11) (171 6) (173 6)
(189 29) (190 8) (191 51) (192 8) (201 5)
(203 15) (204 212) (205 60) (206 19) (216 4)
(217 106) (218 29) (219 13) (221 6) (229 7)
(233 16) (243 29) (244 9) (271 22) (273 12)
(274 4) (305 9) (319 14) (331 6) (332 4)
(360 19) (361 152) (362 56) (363 27)

NAME:12C_2811.2_1160EC39_[895; Isomaltose methoxyamine (8TMS)]
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:281001-10-1
RI:2811
RT:17.476
NUM PEAKS: 89
(73 1000) (74 66) (75 95) (89 31) (101 47)
(103 92) (104 28) (105 26) (109 8) (116 13)
(117 75) (118 9) (129 104) (131 19) (133 36)
(134 8) (143 19) (147 179) (148 39) (150 9)
(157 13) (160 85) (161 45) (164 17) (169 21)
(171 10) (174 10) (189 24) (191 47) (203 10)
(204 304) (205 63) (206 37) (214 12) (217 102)
(218 34) (219 11) (228 18) (230 12) (240 14)
(243 30) (244 8) (245 5) (248 13) (259 11)

(262 9) (271 35) (273 13) (276 11) (287 9)
(304 6) (319 14) (322 10) (325 6) (342 9)
(344 7) (346 8) (352 12) (361 87) (362 45)
(363 21) (365 12) (367 8) (375 12) (395 14)
(396 7) (399 9) (405 5) (407 7) (420 7)
(421 5) (433 12) (436 6) (439 10) (463 11)
(464 16) (468 7) (475 11) (480 10) (482 6)
(486 7) (493 7) (497 16) (506 11) (527 7)
(529 18) (562 11) (564 5) (581 3)

NAME:12C_2518.0_1313EC75_[644; Erythritol (4TMS)]
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:252002-10-1
RI:2518
RT:15.448
NUM PEAKS: 176
(70 13) (71 26) (72 19) (73 1000) (74 84)
(75 108) (76 5) (77 6) (78 3) (79 4)
(80 8) (81 8) (82 13) (83 15) (84 14)
(85 22) (86 8) (87 6) (88 3) (89 43)
(90 4) (91 3) (93 3) (94 4) (95 9)
(96 52) (97 23) (98 28) (99 11) (100 7)
(101 15) (102 7) (103 197) (104 19) (105 13)
(106 4) (107 9) (108 4) (110 4) (111 7)
(112 6) (113 13) (114 8) (115 6) (116 7)
(117 58) (118 6) (119 7) (122 5) (123 11)
(124 3) (125 4) (126 6) (127 6) (128 16)
(129 42) (130 6) (131 19) (132 3) (133 52)
(134 7) (135 11) (136 6) (138 3) (139 3)
(140 7) (141 7) (142 24) (143 13) (144 6)
(145 4) (147 207) (148 32) (149 21) (150 5)
(151 3) (152 4) (153 3) (154 6) (155 7)
(156 99) (157 23) (158 11) (159 3) (160 5)
(161 3) (163 6) (166 3) (167 5) (168 7)
(169 4) (170 21) (171 4) (172 6) (173 36)
(174 4) (175 4) (177 3) (179 3) (180 3)
(181 6) (182 4) (183 5) (184 3) (185 3)
(186 61) (187 11) (188 4) (189 19) (190 5)
(191 8) (192 3) (195 3) (196 3) (197 4)
(198 6) (202 4) (203 3) (204 13) (205 27)
(206 6) (207 6) (209 4) (213 5) (214 51)
(215 8) (216 5) (217 68) (218 14) (219 6)
(221 5) (224 3) (225 13) (226 4) (229 3)
(230 6) (237 6) (244 7) (246 4) (253 3)
(255 3) (258 3) (269 3) (270 3) (274 6)
(275 3) (277 3) (287 3) (291 3) (299 6)
(300 3) (307 6) (313 7) (319 3) (327 4)
(343 14) (344 6) (345 4) (346 10) (347 4)
(355 4) (356 3) (372 3) (373 10) (374 11)
(375 5) (411 3) (414 3) (415 15) (416 11)
(417 9) (444 3) (445 16) (446 65) (447 28)
(448 11)

NAME:12C_2493.1_1313EC75_[657; Erythritol (4TMS)]
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:249001-10-1
RI:2493
RT:15.316
NUM PEAKS: 236
(72 14) (73 1000) (74 83) (75 95) (76 9)

(77 5) (80 5) (82 4) (84 6) (86 3)
(87 14) (88 4) (89 37) (90 4) (93 5)
(94 4) (95 7) (96 35) (97 6) (98 18)
(100 8) (101 16) (102 8) (103 188) (104 15)
(105 12) (106 3) (107 10) (108 5) (114 8)
(115 4) (116 4) (117 51) (118 6) (119 9)
(122 3) (123 9) (124 3) (126 3) (128 14)
(129 39) (130 7) (131 17) (133 43) (134 6)
(135 10) (137 3) (138 3) (139 3) (140 6)
(142 23) (143 12) (144 5) (145 4) (146 4)
(147 218) (148 35) (149 22) (150 5) (151 3)
(152 5) (154 6) (156 74) (157 20) (158 8)
(159 3) (160 5) (161 4) (162 3) (163 5)
(164 4) (166 4) (167 6) (168 6) (170 22)
(171 4) (172 6) (173 39) (174 9) (175 8)
(176 4) (177 3) (179 5) (180 5) (181 5)
(182 4) (184 3) (186 30) (187 8) (188 6)
(189 17) (190 6) (191 10) (192 3) (193 4)
(195 5) (196 7) (198 8) (199 4) (200 5)
(202 4) (203 3) (204 6) (205 27) (206 6)
(207 10) (209 5) (214 23) (215 4) (216 3)
(217 70) (218 15) (219 5) (220 3) (221 14)
(222 3) (223 5) (224 4) (225 11) (226 3)
(227 4) (229 3) (230 4) (231 4) (235 3)
(236 4) (237 5) (239 3) (240 3) (241 3)
(244 5) (246 3) (247 4) (249 4) (250 4)
(251 4) (252 3) (253 5) (254 3) (255 4)
(256 5) (258 5) (263 3) (265 4) (266 5)
(268 4) (269 4) (270 5) (271 3) (273 3)
(274 9) (275 5) (276 3) (277 6) (278 4)
(279 3) (281 6) (283 3) (284 3) (286 4)
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(343 13) (344 8) (345 4) (346 10) (347 6)
(348 3) (349 3) (351 3) (355 5) (356 4)
(362 3) (367 3) (372 3) (373 18) (374 14)
(375 6) (376 4) (378 3) (380 3) (391 3)
(395 3) (398 3) (406 3) (411 3) (412 3)
(414 5) (415 17) (416 12) (417 7) (418 4)
(423 3) (429 3) (430 3) (431 4) (437 4)
(438 3) (442 3) (443 4) (444 3) (445 20)
(446 69) (447 32) (448 13) (449 5) (457 3)
(461 3) (462 3) (468 3) (469 4) (486 3)
(515 3) (522 4) (534 3) (539 3) (540 3)
(543 3)

NAME:12C_2134.7_1274EC17_[904; Galactose methoxyamine (5TMS)]
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:214003-10-1
RI:2135
RT:13.842
NUM PEAKS: 108
(70 5) (72 15) (73 1000) (74 79) (75 66)
(83 16) (84 20) (87 5) (89 48) (90 6)
(92 3) (100 12) (101 13) (102 5) (103 217)
(104 20) (105 11) (112 3) (113 7) (114 10)
(115 6) (116 4) (117 82) (118 8) (119 8)
(120 3) (127 4) (129 97) (130 15) (131 24)

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(133   98) (134   12) (135    8) (138    3) (141    4)
(142    5) (143   12) (147  261) (148   40) (149   23)
(150    3) (155    4) (156    3) (157  111) (158   15)
(159   10) (163   10) (166    4) (171    3) (172   29)
(173   18) (174    5) (175    6) (177    5) (189   29)
(190   11) (191   17) (193    4) (200    3) (201    9)
(202    5) (203    5) (204   27) (205  168) (206   32)
(207   16) (214    3) (216    5) (217  112) (218   23)
(219    9) (227    3) (229   27) (230   11) (231    8)
(232    3) (233    4) (235    4) (243    3) (244    3)
(245    4) (247    3) (257    3) (260    3) (262    8)
(263    7) (268    5) (271    4) (272    4) (273    4)
(274    4) (277    5) (288    4) (291    7) (302    4)
(305    7) (306    5) (307    8) (318    3) (319  217)
(320   68) (321   33) (322    6) (332    6) (333    3)
(378    3) (402    4) (514    4)

NAME:12C_2128.7_1274EC17_[857; Mannitol (6TMS)]
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:213001-10-1
RI:2129
RT:13.804
NUM PEAKS:  237
( 70   18) ( 71   81) ( 72   20) ( 73 1000) ( 74   82)
( 75   77) ( 76    6) ( 77    5) ( 79    3) ( 80    6)
( 81   13) ( 82   15) ( 83   59) ( 84   48) ( 85   60)
( 86    9) ( 87    6) ( 88    6) ( 89   52) ( 90    5)
( 92    3) ( 93   19) ( 94    6) ( 95   12) ( 96    4)
( 97   41) ( 98    8) ( 99   28) (100    7) (101   15)
(102    5) (103  200) (104   21) (105   21) (106    5)
(110    4) (111   25) (112    9) (113   21) (114   28)
(115    9) (116    5) (117   71) (118    7) (119   12)
(120    3) (121    3) (123   11) (125   16) (126    6)
(127   17) (128    5) (129  103) (130   24) (131   25)
(133   66) (134   10) (135   10) (138    4) (139    5)
(140    5) (141   10) (142    9) (143   16) (144    5)
(146   12) (147  261) (148   39) (149   29) (150    4)
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(156    4) (157  112) (158   17) (159    6) (160    3)
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(167    3) (168    5) (169    6) (170    6) (171    3)
(172    8) (173   13) (175    5) (176    3) (177    5)
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(185    4) (186    3) (187    3) (188    5) (189   29)
(190   10) (191   21) (192    6) (198    6) (200    3)
(201    5) (202    8) (203    7) (204   31) (205  167)
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(215    6) (216    7) (217  116) (218   24) (219   11)
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(280    4) (284    3) (288    5) (289    3) (290    4)
(291    9) (292    4) (304    4) (305    6) (306    3)
(307    8) (308    5) (309    3) (311    3) (312    4)
(313    3) (318    6) (319  227) (320   73) (321   31)
(322    7) (323    4) (330    3) (331    5) (332    3)
(333    4) (334    6) (335    4) (336    6) (337    4)
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(338 3) (339 4) (340 3) (342 3) (344 3)
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(512 3) (513 3) (515 3) (516 3) (518 3)
(528 4) (548 3)

NAME:12C_2217.8_1274EC17_9-(Z)-Octadecenoic acid (1TMS)
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:222001-10-1
RI:2218
RT:14.350
NUM PEAKS: 146
(70 43) (71 11) (72 39) (73 838) (74 88)
(75 1000) (76 67) (77 66) (78 11) (79 84)
(80 36) (81 189) (82 96) (83 144) (84 190)
(85 26) (86 9) (87 7) (88 6) (89 27)
(90 3) (91 28) (92 9) (93 49) (94 34)
(95 140) (96 230) (97 128) (98 156) (99 29)
(101 10) (102 3) (103 3) (105 30) (106 8)
(107 27) (108 22) (109 75) (110 86) (111 58)
(112 31) (113 5) (116 27) (117 731) (118 73)
(119 53) (120 8) (121 34) (122 11) (123 57)
(124 37) (125 21) (126 6) (128 5) (129 552)
(130 70) (131 105) (132 135) (133 56) (134 27)
(135 17) (136 6) (137 41) (138 31) (139 11)
(140 4) (141 3) (142 4) (143 38) (144 7)
(145 243) (146 33) (147 35) (148 16) (149 13)
(150 5) (151 26) (152 41) (153 7) (155 26)
(156 7) (157 16) (158 8) (159 20) (160 3)
(161 7) (162 4) (163 4) (164 4) (165 14)
(166 23) (167 8) (168 3) (169 16) (170 9)
(171 26) (172 10) (173 11) (174 5) (175 4)
(179 6) (180 34) (181 6) (183 21) (184 6)
(185 59) (186 14) (187 11) (188 5) (193 4)
(194 5) (199 80) (200 14) (201 13) (206 3)
(207 8) (208 3) (213 11) (214 3) (217 14)
(218 7) (220 10) (221 10) (222 44) (223 9)
(227 4) (235 5) (236 7) (241 8) (246 4)
(255 3) (257 5) (258 3) (264 34) (265 8)
(272 4) (294 4) (295 9) (296 3) (311 3)
(338 3) (339 112) (340 40) (341 9) (354 14)
(355 5)

NAME:12C_2278.6_1274EC17_[583; Erythritol (4TMS)]
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:228001-10-1
RI:2279
RT:14.672
NUM PEAKS: 235
(70 4) (71 45) (72 28) (73 1000) (74 86)
(75 49) (77 27) (78 15) (79 33) (80 21)
(81 24) (85 15) (87 9) (89 27) (91 32)
(92 21) (93 66) (94 12) (98 5) (100 9)
(101 6) (102 3) (103 77) (105 24) (113 5)

(114 8) (117 74) (122 9) (126 10) (128 10)
(129 20) (131 17) (133 131) (134 61) (137 3)
(139 6) (140 7) (142 9) (143 6) (144 5)
(145 4) (147 194) (148 40) (149 18) (150 9)
(151 9) (152 9) (153 6) (154 3) (157 16)
(158 5) (159 8) (163 6) (164 3) (165 7)
(168 7) (170 5) (172 12) (173 12) (176 3)
(180 4) (183 12) (186 13) (188 5) (189 21)
(190 19) (191 12) (194 7) (197 4) (199 11)
(201 34) (202 15) (204 13) (205 45) (206 11)
(212 8) (213 3) (214 21) (215 7) (216 8)
(217 58) (218 19) (219 4) (222 3) (224 5)
(226 15) (227 7) (229 9) (230 4) (231 6)
(233 7) (234 15) (235 8) (236 4) (241 6)
(243 4) (244 9) (245 7) (246 24) (247 8)
(248 6) (251 3) (252 6) (254 13) (256 5)
(257 4) (258 4) (260 11) (265 5) (266 7)
(267 4) (268 12) (269 11) (270 5) (274 3)
(275 9) (278 7) (282 4) (284 10) (285 4)
(286 9) (287 4) (288 3) (289 8) (290 149)
(291 42) (292 18) (293 10) (294 11) (295 3)
(296 6) (301 5) (306 3) (307 4) (308 5)
(310 5) (315 5) (316 6) (317 5) (319 36)
(320 15) (325 6) (327 4) (331 8) (335 3)
(336 5) (346 5) (347 9) (348 5) (352 5)
(354 6) (355 7) (356 4) (359 4) (360 5)
(361 3) (364 6) (365 8) (367 8) (368 4)
(369 4) (374 4) (380 6) (381 3) (382 3)
(383 5) (384 5) (385 6) (387 12) (388 10)
(389 3) (390 5) (392 3) (393 3) (394 3)
(395 3) (404 8) (405 6) (406 3) (409 5)
(410 4) (411 3) (412 7) (413 5) (414 4)
(416 7) (421 7) (422 3) (424 9) (425 9)
(428 3) (430 8) (431 5) (433 6) (434 3)
(437 3) (440 5) (445 4) (448 4) (452 5)
(453 5) (462 4) (465 6) (468 5) (473 4)
(476 4) (477 4) (481 5) (483 3) (486 6)
(489 10) (492 5) (494 3) (498 4) (499 5)
(504 5) (513 4) (521 8) (522 10) (524 3)
(525 10) (530 4) (535 3) (538 7) (539 4)
(541 8) (542 4) (543 3) (545 3) (549 6)
(550 3) (556 6) (567 3) (571 3) (590 3)

NAME:12C_2294.6_1274EC17_[877; beta-D-Galactopyranoside-(1,2)-glycerol (6TMS)]
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:230001-10-1
RI:2295
RT:14.757
NUM PEAKS: 71
(73 1000) (74 70) (75 80) (78 15) (87 12)
(89 11) (101 47) (103 223) (104 21) (116 10)
(117 53) (118 11) (129 115) (130 32) (131 42)
(133 29) (134 15) (135 15) (143 10) (147 207)
(148 42) (149 19) (154 17) (161 9) (163 8)
(189 29) (191 72) (192 19) (202 10) (203 32)
(204 676) (205 142) (206 48) (217 119) (218 42)
(219 50) (223 7) (231 21) (232 10) (240 8)
(242 8) (243 17) (258 6) (274 15) (280 6)
(281 15) (286 8) (293 10) (295 8) (296 13)

(297 9) (298 9) (303 12) (319 14) (324 9)
(331 12) (337 70) (338 25) (359 8) (382 7)
(383 7) (414 10) (450 11) (464 7) (489 18)
(493 16) (494 9) (511 9) (512 13) (574 4)
(579 4)

NAME:12C_2311.4_1274EC17_Galactose-6-phosphate methoxyamine (6TMS)
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:232001-10-1
RI:2311
RT:14.846
NUM PEAKS: 321
(70 43) (71 90) (72 74) (73 1000) (74 112)
(75 212) (76 6) (82 7) (84 27) (86 15)
(87 21) (88 19) (89 37) (90 8) (96 14)
(98 9) (100 24) (101 135) (102 17) (110 10)
(112 21) (113 6) (114 19) (116 13) (124 14)
(129 12) (130 45) (140 6) (144 17) (147 237)
(148 22) (149 11) (150 14) (157 46) (158 27)
(160 159) (162 6) (163 11) (166 3) (168 7)
(169 12) (174 8) (175 8) (177 10) (178 11)
(179 16) (181 13) (182 20) (183 4) (184 6)
(189 5) (191 27) (192 14) (193 13) (195 13)
(196 19) (197 6) (203 4) (204 18) (205 18)
(206 21) (207 35) (208 7) (209 13) (210 5)
(211 39) (212 17) (216 17) (217 23) (218 10)
(220 21) (221 23) (222 21) (223 10) (224 8)
(225 8) (228 13) (229 14) (230 8) (231 21)
(232 10) (233 15) (234 15) (235 8) (238 2)
(242 5) (245 5) (246 10) (247 19) (248 3)
(249 9) (250 15) (251 18) (252 9) (253 17)
(254 14) (255 12) (256 5) (257 10) (258 3)
(261 9) (262 9) (263 15) (264 11) (265 15)
(266 4) (267 9) (270 4) (271 5) (272 8)
(273 3) (274 9) (277 12) (278 4) (279 9)
(280 8) (281 14) (282 10) (283 8) (284 7)
(285 17) (286 9) (287 9) (289 6) (290 5)
(291 10) (292 7) (293 3) (294 6) (295 13)
(297 5) (298 6) (299 130) (300 36) (301 21)
(302 17) (303 18) (304 7) (305 9) (306 7)
(307 8) (308 12) (309 2) (313 6) (314 6)
(316 5) (319 9) (323 9) (324 7) (325 10)
(326 5) (328 161) (329 79) (330 10) (331 29)
(332 3) (336 6) (337 13) (339 8) (340 5)
(341 10) (342 8) (343 8) (345 4) (347 2)
(352 11) (353 6) (354 15) (355 11) (356 4)
(357 51) (358 21) (359 21) (360 6) (362 2)
(363 3) (364 8) (365 5) (368 8) (369 6)
(370 7) (371 18) (373 5) (374 12) (377 10)
(378 4) (379 13) (380 11) (382 12) (386 23)
(387 220) (388 103) (389 47) (390 7) (392 11)
(394 10) (395 11) (396 10) (397 14) (398 8)
(399 3) (402 7) (403 9) (404 14) (405 15)
(406 6) (407 9) (408 4) (412 5) (413 11)
(414 9) (415 4) (416 15) (417 13) (423 8)
(424 11) (425 11) (427 3) (429 12) (433 5)
(434 6) (436 13) (437 7) (438 4) (439 5)
(441 5) (442 4) (443 15) (444 9) (446 10)
(447 5) (448 6) (449 17) (450 6) (451 5)
(452 4) (453 3) (454 9) (455 4) (457 8)

(458 11) (461 10) (462 5) (464 5) (465 8)
(466 9) (469 13) (470 3) (471 21) (472 25)
(473 20) (474 6) (475 3) (476 12) (477 5)
(478 10) (480 5) (483 2) (484 13) (485 11)
(486 5) (487 4) (489 6) (490 10) (491 9)
(492 4) (493 6) (496 14) (498 4) (501 10)
(502 6) (504 18) (505 6) (507 22) (508 10)
(511 8) (514 4) (515 12) (516 3) (518 6)
(522 6) (523 5) (524 2) (525 7) (528 2)
(529 12) (531 2) (532 8) (533 2) (534 4)
(535 4) (538 2) (539 4) (540 6) (541 2)
(542 5) (543 16) (547 5) (549 2) (550 4)
(552 5) (553 3) (559 2) (564 2) (565 2)
(566 5) (568 11) (569 5) (571 2) (572 1)
(574 2) (575 5) (580 3) (581 1) (585 2)
(586 2) (588 4) (590 1) (593 3) (596 2)
(598 1)

NAME:12C_2474.9_1274EC17_[945; Uridine (3TMS)]
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:248002-10-1
RI:2475
RT:15.711
NUM PEAKS: 131
(70 12) (71 8) (72 22) (73 1000) (74 84)
(75 136) (76 9) (77 10) (79 3) (81 8)
(82 6) (83 4) (84 4) (85 13) (86 4)
(87 7) (89 16) (94 3) (95 5) (96 8)
(97 14) (98 5) (99 49) (100 14) (101 28)
(102 7) (103 175) (104 16) (105 9) (110 3)
(111 9) (112 4) (113 19) (114 4) (115 39)
(116 11) (117 29) (118 3) (119 8) (124 4)
(125 5) (126 10) (127 10) (128 4) (129 74)
(130 10) (131 26) (132 4) (133 68) (134 9)
(135 8) (137 3) (138 5) (140 6) (141 7)
(142 7) (143 33) (144 5) (145 8) (147 171)
(148 47) (149 36) (150 5) (151 3) (153 15)
(154 6) (155 6) (156 4) (157 13) (158 3)
(159 5) (163 7) (167 3) (168 11) (169 154)
(170 23) (171 15) (173 3) (174 3) (175 3)
(177 4) (183 12) (184 3) (185 32) (186 5)
(187 3) (189 17) (190 4) (191 46) (192 7)
(203 8) (204 10) (205 4) (211 12) (213 28)
(214 4) (215 17) (216 5) (217 420) (218 102)
(219 45) (220 6) (226 6) (227 5) (229 5)
(230 24) (231 21) (232 5) (239 3) (241 5)
(243 52) (244 11) (245 21) (246 4) (251 3)
(257 7) (258 5) (259 91) (260 20) (261 8)
(265 15) (267 8) (280 3) (299 16) (300 5)
(315 9) (316 3) (317 4) (348 3) (349 3)
(445 5)

NAME:12C_2687.5_1274EC17_[964; Trehalose (8TMS); alpha-D-Glc-(1,1)-alpha-D-Glc]
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:269002-10-1
RI:2688
RT:16.837
NUM PEAKS: 93
(72 12) (73 1000) (74 84) (75 76) (81 20)

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( 94    6) (101   13) (103  160) (104   15) (107    5)
(113    9) (115    8) (116   18) (117   58) (127   10)
(129  146) (130   17) (131   30) (133   53) (135    9)
(142    8) (143   23) (144    8) (145    9) (147  232)
(148   38) (149   31) (153    7) (155   26) (157   26)
(158   10) (163    7) (169  122) (170   19) (171   13)
(177    6) (181    9) (183    6) (189   31) (190   11)
(191  261) (192   40) (193   23) (199    8) (203   13)
(204   84) (205   33) (207   12) (211    5) (217  171)
(218   39) (219   18) (229   14) (230   11) (231   15)
(233    7) (242    4) (243   47) (244   15) (245   10)
(257    6) (258    5) (259    7) (265    4) (271   46)
(272   11) (273    9) (282    3) (287    6) (291    7)
(292    5) (319   16) (320   12) (321    6) (331   23)
(332   13) (361  246) (362   84) (363   42) (364   12)
(374    6) (387    3) (435    7) (451    8) (452    4)
(455    5) (456    3) (461    5) (507    4) (512    4)
(524    4) (528    5) (574    3)
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NAME:12C_2748.2_1274EC17_Trehalose (8TMS); alpha-D-Glc-(1,1)-alpha-D-Glc
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:274002-10-1
RI:2748
RT:17.158
NUM PEAKS:  213
( 70    2) ( 71    3) ( 72   11) ( 73 1000) ( 74   89)
( 75   89) ( 76    5) ( 77    4) ( 79    1) ( 80    1)
( 81   23) ( 82    2) ( 83    5) ( 84    1) ( 85    8)
( 86    1) ( 87    6) ( 88    2) ( 89   15) ( 90    2)
( 91    2) ( 94    1) ( 95    2) ( 97    4) ( 98    1)
( 99    7) (100    1) (101   20) (102    5) (103  243)
(104   23) (105   11) (109   12) (110    1) (111    5)
(112    1) (113   13) (114    4) (115    9) (116   12)
(117   67) (118    7) (119    8) (120    1) (125    1)
(126    1) (127    7) (128    2) (129  192) (130   24)
(131   39) (132    6) (133   52) (134    8) (135    5)
(139    4) (140    1) (141    5) (142    6) (143   26)
(144    4) (145    9) (146    2) (147  287) (148   45)
(149   37) (150    5) (151    3) (153    5) (154    2)
(155   28) (156    6) (157   26) (158    4) (159    5)
(160    1) (161    4) (162    1) (163    6) (164    1)
(165    1) (167    2) (168    1) (169  142) (170   24)
(171   13) (172    2) (173    8) (174    2) (175    5)
(176    1) (177    5) (178    1) (179    1) (181    2)
(182    1) (183    6) (184    1) (185    2) (187    2)
(189   23) (190    7) (191  347) (192   66) (193   31)
(194    4) (195    1) (199    4) (200    1) (201    3)
(202    3) (203   12) (204   98) (205   37) (206   12)
(207    7) (208    1) (215    5) (216    2) (217  177)
(218   47) (219   22) (220    4) (221   12) (222    3)
(223    2) (227    4) (228    2) (229   16) (230   10)
(231   15) (232    5) (233   10) (234    3) (235    1)
(239    1) (241    6) (242    3) (243   59) (244   18)
(245   17) (246    4) (247    5) (248    1) (249    1)
(255    3) (256    1) (257    7) (258    2) (259    6)
(260    2) (261    1) (263    6) (264    1) (265    5)
(266    1) (267    1) (270    1) (271   71) (272   18)
(273   11) (274    2) (275    1) (277    1) (278    1)
(279    7) (280    2) (281    1) (287    2) (288    1)
(289    1) (290    9) (291   12) (292    5) (293    3)
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(303 1) (304 1) (305 9) (306 4) (307 3)
(308 1) (317 4) (318 3) (319 22) (320 11)
(321 5) (322 2) (323 3) (324 1) (331 22)
(332 14) (333 8) (334 3) (335 1) (345 2)
(346 2) (347 1) (360 8) (361 120) (362 66)
(363 29) (364 7) (365 2) (377 3) (378 1)
(379 1) (393 1) (407 1) (408 1) (435 3)
(451 5) (463 2) (464 1)

NAME:12C_2929.8_1274EC17_[902; Melibiose (8TMS); alpha-D-Gal-(1,6)-D-Glc (8TMS)]
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:293001-10-1
RI:2930
RT:18.009
NUM PEAKS: 124
(70 4) (71 5) (72 10) (73 1000) (74 85)
(75 81) (76 4) (77 6) (79 3) (81 20)
(83 6) (85 5) (87 5) (89 8) (97 4)
(99 5) (101 14) (102 4) (103 136) (104 13)
(105 6) (109 7) (111 4) (113 7) (115 5)
(116 11) (117 40) (118 4) (119 5) (127 5)
(129 146) (130 17) (131 28) (132 4) (133 51)
(134 7) (135 5) (139 3) (141 4) (142 4)
(143 27) (144 4) (145 6) (147 276) (148 43)
(149 31) (150 4) (151 3) (153 5) (155 11)
(156 3) (157 19) (158 3) (159 4) (161 5)
(163 4) (169 38) (170 8) (171 6) (173 4)
(175 5) (177 6) (181 3) (183 4) (189 26)
(190 10) (191 223) (192 39) (193 18) (201 3)
(203 12) (204 808) (205 166) (206 70) (207 18)
(208 3) (215 5) (217 159) (218 37) (219 17)
(220 3) (221 21) (222 5) (223 3) (229 6)
(230 24) (231 14) (232 4) (233 5) (239 3)
(242 3) (243 25) (244 7) (245 7) (246 3)
(255 3) (257 4) (265 6) (271 14) (272 3)
(291 9) (292 3) (293 9) (295 3) (304 6)
(305 24) (306 9) (307 4) (317 4) (318 14)
(319 12) (320 4) (331 5) (332 8) (333 4)
(343 7) (344 3) (345 5) (361 29) (362 11)
(363 5) (433 16) (434 8) (435 5)

NAME:12C_3337.9_1191EC10_[700; Ergosta-5,7-dien-3-ol]
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:334001-10-1
RI:3338
RT:19.741
NUM PEAKS: 90
(70 66) (71 155) (73 1000) (74 85) (75 887)
(76 70) (77 108) (81 244) (83 108) (89 18)
(90 13) (91 157) (93 130) (94 21) (95 155)
(97 52) (100 17) (101 47) (105 118) (107 68)
(109 72) (111 20) (115 78) (116 29) (117 80)
(119 132) (121 45) (123 21) (128 65) (129 198)
(130 44) (131 160) (132 32) (133 57) (135 27)
(141 57) (142 37) (143 165) (144 73) (145 129)
(146 37) (149 20) (151 19) (153 20) (154 14)
(155 91) (156 31) (157 88) (158 51) (159 85)
(160 12) (161 29) (165 29) (167 18) (168 15)
(169 55) (170 21) (171 63) (172 18) (173 27)

(180 10) (181 27) (183 45) (185 40) (187 18)
(193 28) (195 21) (196 16) (197 51) (200 16)
(201 23) (207 44) (211 52) (212 17) (213 24)
(221 58) (222 21) (225 17) (239 25) (242 13)
(251 17) (253 20) (339 51) (340 23) (341 12)
(365 61) (366 22) (371 12) (380 20) (471 14)

NAME:12C_3350.3_1274EC11_[692; Ergosta-7,22-dien-3-ol (1TMS)]
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:335001-10-1
RI:3350
RT:19.858
NUM PEAKS: 159
(70 48) (73 599) (74 60) (75 1000) (76 89)
(77 162) (78 65) (79 292) (80 38) (81 278)
(82 29) (83 118) (86 22) (87 26) (89 39)
(91 298) (92 55) (93 223) (94 59) (95 174)
(97 22) (101 35) (103 68) (104 19) (105 281)
(106 53) (107 280) (108 54) (109 83) (114 26)
(115 103) (116 23) (117 131) (118 13) (119 152)
(120 50) (121 120) (123 41) (124 36) (127 26)
(128 36) (129 110) (130 34) (131 159) (132 59)
(133 144) (134 47) (135 55) (141 29) (142 34)
(143 77) (144 28) (145 154) (146 67) (147 254)
(148 44) (149 55) (150 97) (151 23) (153 18)
(155 48) (156 20) (157 86) (159 143) (160 45)
(161 49) (164 58) (169 63) (171 75) (172 24)
(173 62) (174 22) (175 33) (177 21) (183 35)
(185 62) (186 29) (187 32) (188 13) (189 37)
(195 18) (197 23) (199 45) (201 33) (202 27)
(203 22) (205 22) (209 30) (210 18) (211 70)
(213 92) (216 21) (219 16) (220 20) (222 22)
(226 19) (227 91) (228 27) (232 15) (239 22)
(241 14) (248 20) (251 20) (253 101) (254 25)
(267 24) (281 50) (282 33) (283 22) (284 17)
(290 13) (295 17) (301 20) (303 11) (307 21)
(314 16) (315 18) (321 12) (329 21) (330 16)
(342 17) (343 272) (344 122) (345 40) (360 15)
(365 25) (366 16) (371 35) (372 25) (375 15)
(378 23) (380 18) (386 91) (387 55) (388 25)
(389 13) (404 21) (417 18) (433 20) (443 15)
(444 16) (446 14) (455 37) (456 14) (457 13)
(470 22) (471 19) (481 13) (486 17) (492 13)
(504 18) (509 13) (513 16) (520 16) (545 7)
(546 11) (569 9) (580 5) (592 4)

NAME:12C_3358.2_1191EC08_[693; Ergost-7-en-3-ol (1TMS)]
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:335002-10-1
RI:3358
RT:19.826
NUM PEAKS: 48
(71 242) (73 477) (75 1000) (76 93) (79 205)
(81 185) (83 74) (91 269) (92 92) (93 167)
(94 47) (95 217) (96 51) (97 68) (105 281)
(106 64) (107 179) (108 54) (109 80) (111 23)
(117 104) (119 154) (120 45) (121 86) (123 35)
(128 32) (131 153) (133 113) (134 43) (143 40)
(145 123) (147 174) (159 82) (161 67) (173 29)
(201 39) (213 147) (214 40) (229 53) (255 159)

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(256   39) (273   19) (306   27) (307   19) (367   21)
(471   15) (472   68) (473   40)

NAME:12C_3401.9_1274EC11_[805; 4,4-Dimethylcholesta-8,24-dien-3-ol (1TMS)]
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:340002-10-1
RI:3402
RT:20.078
NUM PEAKS:  112
( 73 1000) ( 74   69) ( 75  649) ( 79  223) ( 81  364)
( 82   80) ( 87   36) ( 89   31) ( 91  278) ( 92   47)
( 93  269) ( 94   53) ( 95  377) (104   17) (105  290)
(106   59) (107  286) (108   56) (109  265) (117  147)
(119  264) (120   73) (121  183) (122   80) (123  130)
(124   31) (128   35) (129  273) (131  178) (132  120)
(133  228) (134  116) (135  775) (136  181) (137   84)
(143  115) (144   54) (145  235) (146  128) (148   68)
(149  188) (150   29) (152   34) (154   12) (156   29)
(157  112) (158   33) (159  149) (160   66) (161  137)
(162   40) (163   85) (169   26) (171  101) (172   31)
(173  126) (174   75) (175  140) (176   38) (177   50)
(183   41) (185   67) (186   29) (187  144) (188   61)
(189   58) (190   29) (197   24) (199   61) (200   17)
(201   49) (203   58) (211   62) (213   30) (215   48)
(216   29) (225   69) (226   29) (229   50) (231   16)
(241  113) (242   20) (243   65) (255   23) (257   36)
(258   80) (259   27) (260    9) (278   14) (295   39)
(296   27) (325   24) (326   23) (351   42) (366   12)
(379   87) (380   53) (394   47) (396   17) (402   21)
(467   15) (471   30) (474   11) (484   76) (485   71)
(486   22) (491   23) (513   31) (540   16) (571    8)
(590    9) (592    4)

NAME:12C_3487.5_1191EC08_[568; 2,3-Dihexadecanoylglycerol (1TMS)]
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:349001-10-1
RI:3488
RT:20.373
NUM PEAKS:  103
( 70   57) ( 73 1000) ( 74   42) ( 75  286) ( 79  113)
( 81   88) ( 83  102) ( 84   41) ( 86    8) ( 91   29)
( 95  138) ( 97   49) ( 98   64) (101   46) (102   23)
(103  242) (104   27) (105   18) (106   20) (107   20)
(109  105) (115   33) (116   21) (117   84) (123   15)
(126    7) (128   25) (129  629) (130   84) (131  115)
(134   12) (135   41) (139    9) (142   13) (143   19)
(145  456) (146   66) (147   26) (148   11) (149   32)
(157   22) (159    9) (167   11) (168   21) (173   28)
(174   10) (178   15) (182   18) (183  122) (184    7)
(189   37) (193   33) (194   27) (201   27) (208    6)
(219   29) (220   19) (224   24) (227    5) (237   13)
(239   16) (243    5) (255    9) (257  194) (258   35)
(259   19) (273   57) (274   16) (275   15) (277    9)
(295   14) (296   10) (297    9) (300    7) (311   13)
(312   13) (313  100) (314   16) (315   23) (327   25)
(328   14) (329   30) (347    6) (348    6) (371   18)
(384   11) (385   32) (390    5) (409   17) (424   11)
(428    6) (433   28) (434   31) (469   11) (474   12)
(538    7) (551   18) (556    6) (569   17) (572   15)
(578   18) (579   10) (586    8)
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NAME:12C_3301.9_1274EC11_[674; Ergosterol (1TMS)]
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:331001-10-1
RI:3302
RT:19.651
NUM PEAKS: 335

(70 165)	(71 742)	(72 81)	(73 1000)	(74 130)
(75 788)	(76 91)	(77 121)	(79 95)	(80 18)
(81 367)	(82 46)	(83 329)	(84 153)	(85 340)
(86 21)	(87 23)	(88 3)	(89 52)	(90 27)
(91 132)	(93 113)	(95 285)	(96 79)	(97 133)
(98 50)	(99 141)	(100 43)	(101 51)	(102 27)
(103 261)	(104 11)	(105 102)	(106 47)	(107 82)
(108 11)	(109 80)	(110 36)	(111 44)	(112 34)
(113 76)	(115 111)	(116 69)	(117 198)	(118 39)
(119 107)	(120 25)	(121 73)	(122 20)	(123 42)
(124 23)	(125 63)	(126 31)	(127 63)	(128 71)
(129 969)	(130 185)	(131 357)	(132 69)	(133 123)
(135 25)	(136 25)	(137 58)	(139 27)	(140 3)
(141 134)	(142 73)	(143 198)	(144 70)	(145 990)
(146 151)	(147 55)	(151 5)	(152 30)	(153 30)
(154 64)	(155 379)	(156 70)	(157 204)	(158 62)
(159 138)	(160 43)	(161 18)	(162 9)	(163 7)
(165 53)	(166 13)	(167 48)	(168 24)	(169 114)
(170 29)	(171 93)	(172 35)	(173 17)	(174 6)
(176 13)	(177 11)	(178 16)	(180 26)	(181 83)
(182 38)	(183 98)	(184 31)	(185 62)	(187 24)
(188 42)	(189 74)	(190 16)	(191 21)	(193 6)
(194 10)	(195 76)	(196 37)	(197 79)	(198 22)
(199 72)	(200 25)	(201 35)	(207 26)	(209 42)
(210 45)	(211 89)	(212 32)	(213 76)	(214 40)
(215 25)	(216 12)	(218 18)	(219 7)	(222 16)
(223 37)	(224 24)	(225 27)	(226 14)	(227 37)
(228 25)	(229 376)	(230 86)	(231 27)	(232 7)
(235 15)	(237 52)	(238 33)	(239 53)	(240 18)
(241 3)	(243 9)	(245 31)	(246 22)	(247 16)
(248 16)	(250 9)	(251 33)	(252 16)	(253 126)
(254 39)	(255 27)	(257 11)	(259 17)	(260 9)
(261 12)	(264 8)	(266 15)	(267 5)	(268 3)
(271 21)	(274 19)	(275 24)	(276 20)	(277 35)
(278 21)	(279 16)	(280 5)	(283 15)	(285 9)
(286 9)	(291 17)	(292 6)	(293 10)	(294 4)
(297 7)	(298 10)	(299 11)	(300 7)	(301 71)
(302 27)	(303 7)	(305 6)	(306 8)	(307 40)
(308 21)	(309 6)	(313 97)	(314 40)	(315 8)
(319 10)	(320 10)	(322 18)	(323 12)	(325 9)
(326 13)	(327 37)	(328 20)	(329 29)	(330 16)
(332 14)	(333 36)	(334 6)	(336 13)	(337 64)
(338 16)	(341 21)	(345 5)	(346 18)	(347 10)
(348 10)	(349 3)	(350 14)	(351 7)	(352 24)
(353 11)	(359 3)	(360 14)	(361 15)	(362 25)
(363 81)	(364 24)	(365 3)	(366 10)	(367 13)
(370 3)	(371 5)	(373 11)	(377 17)	(378 31)
(379 5)	(380 12)	(381 19)	(382 5)	(383 27)
(384 16)	(385 27)	(386 7)	(388 3)	(391 14)
(395 13)	(397 11)	(401 13)	(402 3)	(408 6)
(409 4)	(410 18)	(414 3)	(417 7)	(422 16)
(425 7)	(426 21)	(427 21)	(429 5)	(432 10)
(439 12)	(440 27)	(442 11)	(443 9)	(446 11)

(447 13) (449 21) (450 29) (453 3) (456 6)
(459 6) (463 3) (465 12) (466 42) (467 25)
(468 38) (469 35) (470 5) (471 14) (472 15)
(473 4) (475 31) (476 24) (480 13) (489 23)
(490 4) (491 8) (494 5) (495 20) (497 14)
(498 8) (500 16) (501 3) (502 7) (503 25)
(508 7) (509 12) (511 5) (512 8) (514 16)
(515 10) (516 10) (518 11) (521 17) (522 15)
(524 12) (525 11) (526 4) (527 4) (528 13)
(535 26) (538 4) (540 16) (542 14) (543 21)
(544 17) (545 5) (550 3) (551 5) (553 4)
(556 10) (559 5) (564 3) (569 5) (573 3)
(575 7) (580 10) (583 9) (585 6) (589 9)
(590 10) (593 5) (595 4) (597 5) (598 7)

NAME:12C_3183.2_1160EC23_[748; D-Sedoheptulose-7-phosphate (7TMS)]
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:318001-10-1
RI:3183
RT:19.137
NUM PEAKS: 111
(72 7) (73 1000) (74 84) (81 30) (85 8)
(87 4) (101 10) (103 105) (104 6) (109 15)
(113 17) (116 8) (117 37) (118 5) (127 6)
(129 140) (130 16) (131 26) (132 7) (133 54)
(134 7) (135 6) (141 4) (142 8) (143 24)
(145 8) (147 322) (148 49) (149 36) (151 3)
(153 7) (155 28) (156 4) (157 15) (169 46)
(170 8) (171 9) (173 6) (175 4) (181 3)
(183 10) (189 26) (191 38) (199 4) (203 7)
(204 42) (205 20) (206 6) (208 14) (209 9)
(211 33) (212 4) (213 4) (217 93) (218 21)
(219 10) (225 5) (227 14) (228 4) (231 9)
(233 5) (242 23) (243 45) (244 13) (245 10)
(253 4) (255 4) (257 4) (269 3) (270 22)
(271 200) (272 50) (273 21) (291 7) (293 3)
(294 3) (298 6) (299 80) (300 22) (301 11)
(302 4) (305 7) (314 10) (315 225) (316 65)
(317 34) (318 8) (319 7) (341 11) (343 6)
(357 11) (358 5) (360 3) (361 32) (362 12)
(363 6) (372 4) (386 10) (387 78) (388 33)
(389 18) (422 3) (423 23) (424 5) (431 3)
(454 3) (484 3) (512 6) (513 32) (514 20)
(515 10)

NAME:12C_2723.7_1160EC23_[777; Fructose-6-phosphate methoxyamine (6TMS)]
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:272001-10-1
RI:2724
RT:17.023
NUM PEAKS: 75
(73 1000) (74 78) (89 58) (90 7) (91 10)
(101 64) (121 7) (127 7) (129 155) (133 57)
(135 29) (140 9) (142 112) (143 18) (151 18)
(165 5) (173 74) (174 38) (180 8) (181 18)
(193 12) (195 26) (207 20) (211 84) (212 11)
(214 6) (217 158) (218 22) (225 66) (226 14)
(227 23) (228 14) (236 16) (269 10) (283 16)
(285 12) (298 13) (299 334) (300 83) (301 35)
(313 14) (314 19) (315 343) (316 95) (317 41)

(318 10) (328 5) (341 8) (342 5) (354 20)
(357 43) (358 13) (379 3) (386 35) (387 255)
(388 100) (389 56) (390 11) (394 6) (410 3)
(414 13) (449 5) (451 15) (453 6) (454 3)
(459 21) (460 6) (461 9) (474 5) (542 5)
(543 4) (544 10) (545 9) (546 6) (558 3)

NAME:12C_2578.1_1274EC11_[734; 1-Monooleoylglycerol (2TMS); 1-Monohexadecenoylglycerol (1TMS)]
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:258001-10-1
RI:2578
RT:16.266
NUM PEAKS: 108
(70 43) (71 35) (72 24) (73 1000) (74 89)
(75 313) (76 15) (77 38) (79 66) (80 23)
(81 185) (82 42) (83 124) (84 32) (85 27)
(89 40) (91 22) (93 50) (94 18) (95 108)
(96 33) (97 79) (98 48) (99 32) (100 8)
(101 139) (102 18) (103 308) (104 30) (105 33)
(106 6) (107 31) (108 14) (109 50) (110 12)
(111 45) (112 12) (113 24) (115 23) (116 79)
(117 133) (118 20) (119 31) (120 14) (121 53)
(122 10) (123 40) (124 6) (125 16) (129 580)
(130 102) (131 154) (132 49) (133 124) (134 27)
(135 67) (136 17) (137 35) (139 10) (145 52)
(146 40) (147 444) (148 75) (149 84) (150 14)
(151 20) (152 7) (153 13) (159 6) (161 9)
(162 4) (163 24) (165 16) (171 6) (175 20)
(176 9) (187 14) (188 19) (192 9) (201 90)
(202 20) (203 127) (205 58) (206 10) (215 23)
(219 34) (220 6) (221 14) (236 15) (237 53)
(238 12) (243 7) (244 7) (255 6) (257 40)
(258 20) (272 5) (279 22) (286 13) (311 11)
(339 7) (369 106) (370 46) (371 17) (382 19)
(457 17) (458 14) (475 3)

NAME:12C_2386.9_1160EC23_[928; Glucopyranose-6-phosphate (6TMS)]
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:239001-10-1
RI:2387
RT:15.242
NUM PEAKS: 78
(72 12) (73 1000) (74 84) (75 100) (81 17)
(87 3) (99 4) (101 20) (111 6) (113 18)
(115 6) (116 9) (127 4) (129 153) (130 15)
(131 24) (133 58) (134 6) (135 9) (143 15)
(147 180) (148 25) (149 21) (151 5) (155 10)
(161 4) (169 10) (181 6) (189 25) (190 5)
(191 46) (192 7) (193 8) (195 5) (204 221)
(205 43) (206 16) (207 12) (208 3) (211 37)
(212 5) (217 57) (219 5) (225 9) (227 9)
(231 5) (242 5) (243 12) (247 6) (253 4)
(269 5) (270 7) (271 18) (272 4) (283 3)
(285 3) (298 4) (299 110) (300 29) (301 14)
(314 4) (315 40) (316 11) (317 8) (345 8)
(357 36) (358 11) (359 5) (369 3) (370 20)
(371 7) (372 3) (373 3) (386 14) (387 120)
(388 48) (389 28) (390 7)

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NAME:12C_2310.0_1191EC10_Fructose-6-phosphate methoxyamine (6TMS)
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:232002-10-1
RI:2310
RT:14.783
NUM PEAKS:  127
( 70    8) ( 71   11) ( 72   15) ( 73 1000) ( 74   90)
( 75   89) ( 76    4) ( 77    8) ( 81    4) ( 82    3)
( 83    7) ( 84   28) ( 85   11) ( 87    4) ( 88    3)
( 89   47) ( 90    5) ( 91    4) ( 93    3) ( 95    3)
( 97    5) ( 98    4) ( 99    6) (100    7) (101   32)
(102    6) (103   73) (104    9) (105    6) (111    4)
(113    7) (114   11) (115    9) (116   11) (117   21)
(118    3) (119    7) (126    5) (127    5) (128    3)
(129   65) (130    7) (131   18) (132    3) (133   56)
(134    7) (135   11) (137    3) (141    3) (142    5)
(143    7) (147  129) (148   21) (149   14) (151    4)
(152    4) (155    4) (156    4) (157    5) (159    3)
(163    5) (169    4) (172    5) (173    5) (180    3)
(181    6) (182    4) (183    3) (189    7) (190    3)
(191   11) (193    6) (195    7) (196    3) (197    3)
(204   10) (205    8) (206    3) (207   11) (208    3)
(209    4) (211   29) (212    6) (213    3) (214    3)
(217   81) (218   19) (219    7) (221    5) (225   11)
(226    3) (227    8) (232    4) (243    5) (244    4)
(245    4) (260    3) (270    3) (271    3) (283    3)
(285    5) (286    3) (298    5) (299   64) (300   23)
(301   11) (302    4) (313    3) (314    8) (315  105)
(316   31) (317   15) (318    5) (319    3) (341    5)
(342    3) (355    3) (356    4) (357   15) (358    5)
(359    3) (373    3) (403    5) (458    3) (459    9)
(460    4) (461    3)

NAME:12C_2257.2_1160EC23_[715; Erythritol (4TMS)]
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:226001-10-1
RI:2257
RT:14.556
NUM PEAKS:  143
( 70   24) ( 72   14) ( 73 1000) ( 74   61) ( 75   94)
( 76    5) ( 80    4) ( 82   13) ( 83    9) ( 84  290)
( 85   22) ( 86   22) ( 88    3) ( 89   36) ( 90    3)
( 94    4) ( 96    3) ( 99    8) (100   17) (101    8)
(102    8) (103  227) (104   20) (105   11) (108    3)
(111   12) (112    3) (113    7) (114    8) (115    4)
(116   24) (117   66) (118    8) (119    6) (123    3)
(126    3) (127    3) (128   11) (129   34) (130   10)
(131   18) (132    6) (133   45) (134    5) (135    6)
(140    4) (141    6) (142   33) (143   20) (144   43)
(145    9) (146    4) (147  210) (148   32) (149   20)
(153    3) (154    3) (155    4) (157   12) (158   11)
(159    4) (161    3) (163    4) (167    4) (168    6)
(169    3) (170    7) (171    4) (172   14) (173   15)
(174   53) (175   11) (176    3) (180    3) (182    4)
(183    8) (184    3) (186   11) (187    5) (188    5)
(189   18) (190    3) (191    9) (198    3) (200    7)
(201    8) (202   30) (203    6) (204   13) (205   31)
(206    7) (207    3) (213    6) (214    5) (216    3)
(217   93) (218   20) (219    7) (221    4) (225   12)
(226    3) (232    3) (242    5) (243    3) (244    4)
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(256 5) (257 9) (258 4) (260 3) (268 4)
(269 3) (270 4) (271 5) (277 6) (300 3)
(307 9) (308 3) (316 3) (330 12) (331 8)
(332 3) (342 5) (343 4) (367 4) (372 3)
(373 34) (374 19) (375 8) (376 3) (403 4)
(404 3) (437 4) (447 9) (448 6) (457 4)
(476 3) (477 3) (547 7) (548 6) (550 3)
(551 7) (552 6) (553 3)

NAME:12C_2718.4_1313EC43_[824; D-Sedoheptulose-7-phosphate (7TMS)]
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:272002-10-1
RI:2718
RT: 16.521
NUM PEAKS: 469
(70 2) (72 15) (73 1000) (74 86) (75 58)
(76 3) (77 6) (79 1) (80 1) (81 6)
(82 6) (84 2) (86 3) (87 6) (88 3)
(89 24) (90 3) (91 3) (92 2) (93 3)
(94 2) (95 1) (96 2) (98 4) (100 6)
(101 39) (102 6) (103 47) (104 6) (105 10)
(106 3) (107 7) (108 2) (109 4) (110 1)
(111 4) (112 2) (113 7) (114 6) (115 11)
(116 18) (117 22) (118 3) (119 8) (120 2)
(121 6) (122 3) (123 3) (124 3) (125 1)
(126 3) (127 3) (128 4) (129 113) (130 16)
(131 22) (132 7) (133 62) (134 9) (135 18)
(136 4) (137 11) (138 4) (139 3) (140 4)
(141 1) (142 25) (143 12) (144 3) (145 7)
(146 2) (147 132) (148 23) (149 16) (150 3)
(151 9) (152 3) (153 4) (154 4) (155 8)
(156 5) (157 10) (158 5) (159 4) (160 12)
(161 10) (162 2) (163 7) (164 2) (165 4)
(166 4) (167 4) (168 5) (169 13) (170 6)
(171 6) (172 4) (173 25) (174 5) (175 5)
(176 2) (177 2) (178 2) (179 4) (180 7)
(181 12) (182 6) (183 7) (184 3) (185 3)
(186 3) (187 2) (188 2) (189 16) (190 6)
(191 104) (192 18) (193 19) (194 4) (195 12)
(196 8) (197 5) (198 4) (199 8) (200 4)
(201 2) (202 2) (203 5) (204 103) (205 19)
(206 7) (207 18) (208 5) (209 7) (210 5)
(211 58) (212 10) (213 7) (214 2) (215 4)
(216 4) (217 121) (218 31) (219 15) (220 2)
(221 3) (222 1) (223 1) (224 2) (225 25)
(226 6) (227 16) (228 7) (229 4) (230 4)
(231 6) (232 2) (233 2) (234 2) (235 1)
(236 8) (237 2) (238 1) (239 1) (240 3)
(241 5) (242 4) (243 16) (244 3) (245 3)
(246 1) (247 4) (248 1) (249 1) (250 2)
(251 2) (252 2) (253 4) (254 4) (255 4)
(256 2) (257 3) (258 2) (259 4) (260 2)
(261 3) (262 1) (263 1) (264 2) (265 2)
(266 3) (267 3) (268 5) (269 5) (270 5)
(271 5) (272 4) (273 2) (274 2) (275 2)
(276 1) (277 3) (278 2) (279 2) (280 1)
(281 1) (282 3) (283 7) (284 4) (285 8)
(286 4) (287 2) (289 4) (290 2) (291 3)
(292 3) (294 1) (295 1) (297 2) (298 12)
(299 132) (300 41) (301 20) (302 3) (303 2)

(304 4) (305 6) (306 4) (307 3) (308 2)
(309 2) (310 1) (311 2) (312 2) (313 4)
(314 14) (315 128) (316 36) (317 20) (318 5)
(320 1) (322 2) (323 1) (325 1) (326 1)
(327 2) (328 2) (329 3) (330 3) (331 2)
(332 2) (335 2) (337 1) (339 2) (340 2)
(341 6) (342 2) (343 2) (345 3) (346 2)
(347 1) (348 3) (349 2) (350 1) (351 1)
(352 3) (353 4) (354 12) (355 5) (356 7)
(357 21) (358 8) (359 4) (360 5) (361 29)
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(389 15) (390 4) (391 1) (392 2) (393 2)
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(523 2) (524 1) (525 3) (526 2) (527 3)
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(536 1) (537 1) (538 3) (539 2) (540 2)
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(546 2) (547 1) (548 2) (549 1) (550 1)
(551 1) (553 1) (554 1) (555 1) (556 2)
(557 1) (558 1) (559 1) (560 1) (561 1)
(562 1) (563 1) (564 1) (565 1) (566 1)
(571 1) (572 1) (573 1) (574 1) (575 1)
(577 1) (578 1) (581 1) (588 1)

NAME:12C_2347.2_1313EC43_Glucose-6-phosphate methoxyamine (BP) (6TMS)
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:235002-10-1
RI:2347
RT: 14.555
NUM PEAKS: 146
(72 15) (73 1000) (74 81) (75 103) (76 7)
(77 11) (79 7) (80 3) (81 6) (86 4)
(87 4) (88 3) (89 46) (90 5) (91 8)
(92 2) (93 3) (95 4) (97 3) (98 3)

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(100    8) (101   37) (102    9) (103   48) (104    4)
(105   14) (106    5) (107    3) (108    2) (109    2)
(114    8) (115   11) (116   19) (118    2) (119    8)
(121    3) (129   69) (130   16) (131   30) (133   66)
(134   10) (135   14) (136    2) (137    4) (138    2)
(142    2) (143   11) (144    2) (145    7) (146    2)
(147  132) (148   19) (149   18) (150    4) (151    5)
(154    2) (157   32) (158    4) (159    6) (160   38)
(161   13) (162    2) (163    5) (172    2) (173    3)
(174    2) (175    2) (176    2) (177    2) (180    2)
(181    6) (188    1) (189    8) (190    1) (191   14)
(192    3) (193    8) (194    2) (195    4) (197    2)
(201    3) (203    5) (204    7) (205    8) (207   16)
(211   38) (212    6) (213    5) (215    2) (216    3)
(217   30) (218    6) (225   10) (226    2) (227    8)
(228    5) (229    4) (230    3) (231    2) (241    3)
(243    5) (244    3) (245    2) (247    8) (253    3)
(265    1) (268    2) (269    5) (270    1) (278    1)
(283    3) (285    4) (298    8) (299   92) (300   26)
(301   11) (314    9) (315   43) (316   12) (317    6)
(318    1) (319    2) (331    4) (332    2) (341    4)
(356    6) (357   27) (358    8) (359    3) (370    2)
(373    3) (374    2) (385    2) (386   27) (387  101)
(388   39) (389   19) (390    3) (409    1) (435    1)
(470    4) (471    9) (472    3) (473    3) (501    2)
(569    1)

NAME:12C_2039.0_1313EC43_[607; Putrescine (4TMS)]
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:204003-10-1
RI:2039
RT: 12.763
NUM PEAKS:  219
( 70   80) ( 71  135) ( 72   41) ( 73  616) ( 74  121)
( 75  287) ( 76    2) ( 79   19) ( 80   11) ( 81   17)
( 82    3) ( 83   22) ( 84  132) ( 85  103) ( 86  256)
( 87   53) ( 88   26) ( 93   10) ( 94    4) ( 95    7)
( 96    3) ( 98   29) ( 99  150) (100  259) (101    1)
(102   49) (108    1) (110   49) (111    4) (112   71)
(113   21) (114   42) (115    4) (116   31) (122    9)
(123   11) (124   12) (125    2) (126  152) (127   44)
(128    7) (130  106) (131   25) (140   26) (141    9)
(142  128) (143   10) (146   57) (147  116) (148   31)
(150    4) (152    9) (153    7) (154   21) (155   10)
(156    5) (157    5) (158   12) (160  252) (161    1)
(162    7) (164    5) (166    9) (167   14) (168    5)
(169    1) (170    3) (172  112) (173    4) (174  407)
(175   51) (176   45) (179   18) (180    6) (181   13)
(182    4) (183    5) (185    2) (186   34) (188   24)
(194    5) (197    7) (198    9) (200  118) (201   19)
(204  129) (207   10) (208    9) (210    3) (212    6)
(213    5) (214 1000) (215  205) (216   97) (231    9)
(232    4) (233    3) (239    9) (240   12) (241    4)
(242    1) (245    3) (246   28) (250    6) (251    3)
(252   12) (253    1) (257    3) (258   13) (259    2)
(261    5) (266   11) (267    5) (268   27) (269   18)
(270    5) (272    3) (276    1) (280    7) (281    1)
(282    3) (283   12) (287    5) (288   49) (289   13)
(291   11) (292   21) (295    3) (305    1) (311   17)
(319   30) (320    4) (321    6) (324    2) (325    5)
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(330 9) (331 2) (332 2) (334 4) (336 7)
(339 17) (352 9) (353 2) (355 15) (356 10)
(358 1) (360 1) (361 6) (363 2) (367 1)
(372 14) (374 8) (375 61) (376 48) (377 18)
(381 3) (395 14) (398 2) (407 2) (412 2)
(416 2) (420 2) (425 8) (430 3) (435 1)
(439 2) (443 1) (444 3) (448 8) (452 4)
(454 2) (455 2) (456 6) (457 9) (458 6)
(461 4) (462 8) (465 4) (467 7) (469 3)
(471 4) (474 12) (475 21) (476 9) (478 13)
(479 5) (482 4) (483 6) (484 6) (488 5)
(489 3) (493 15) (494 2) (497 15) (501 10)
(502 2) (504 1) (505 4) (506 2) (513 7)
(525 2) (526 3) (527 7) (530 7) (538 1)
(547 2) (550 4) (552 7) (563 3) (566 1)
(571 2) (575 11) (580 5) (583 6) (586 5)
(589 2) (590 1) (592 6) (595 4)

NAME:12C_1476.2_1313EC75_Citramalic acid (3TMS)
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:148001-10-1
RI:1476
RT: 8.471
NUM PEAKS: 38
(73 1000) (74 89) (75 222) (76 14) (85 40)
(86 6) (115 117) (116 15) (117 41) (131 33)
(133 83) (134 10) (143 17) (144 8) (147 404)
(148 65) (149 70) (150 8) (151 5) (157 14)
(163 29) (164 5) (185 18) (190 8) (203 33)
(205 6) (219 3) (221 14) (231 32) (233 26)
(247 141) (248 31) (259 33) (260 7) (261 4)
(321 16) (322 6) (349 10)

NAME:12C_1735.8_1313EC75_Glycerol-2-phosphate (4TMS)
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:174002-10-1
RI:1736
RT: 10.585
NUM PEAKS: 393
(70 9) (71 14) (72 24) (73 1000) (74 81)
(75 224) (76 10) (77 18) (78 7) (79 14)
(80 4) (81 5) (82 4) (83 5) (84 16)
(85 11) (86 7) (87 13) (88 4) (89 25)
(90 4) (91 8) (92 6) (93 7) (94 5)
(95 5) (96 5) (97 9) (98 6) (99 10)
(100 10) (101 93) (102 12) (103 111) (104 10)
(105 15) (106 9) (107 4) (108 1) (109 3)
(110 4) (111 6) (112 2) (113 11) (114 6)
(115 21) (116 55) (117 43) (118 11) (119 9)
(120 3) (121 6) (122 2) (123 7) (124 3)
(125 1) (126 2) (127 6) (128 3) (129 114)
(130 15) (131 43) (132 5) (133 84) (134 16)
(135 15) (136 3) (137 9) (138 5) (139 4)
(140 5) (141 11) (142 8) (143 10) (144 2)
(145 1) (146 4) (147 224) (148 39) (149 30)
(150 5) (151 7) (152 4) (153 56) (154 9)
(155 8) (156 1) (157 10) (159 27) (160 9)
(161 4) (162 1) (163 8) (166 3) (167 12)
(168 5) (169 10) (170 8) (171 5) (174 7)
(175 5) (176 3) (177 8) (178 1) (179 3)

(180	6)	(181	10)	(182	3)	(183	6)	(184	1)
(185	3)	(186	3)	(187	5)	(188	4)	(189	16)
(190	6)	(191	17)	(192	7)	(193	14)	(194	6)
(195	9)	(196	1)	(197	4)	(198	1)	(199	1)
(200	3)	(201	1)	(203	6)	(204	33)	(205	23)
(206	3)	(207	24)	(210	3)	(211	90)	(212	20)
(213	10)	(214	1)	(215	4)	(216	1)	(217	61)
(218	20)	(219	8)	(220	4)	(221	2)	(222	3)
(223	2)	(225	6)	(226	4)	(227	20)	(228	5)
(229	5)	(230	3)	(231	16)	(232	8)	(233	3)
(234	3)	(235	4)	(236	1)	(237	5)	(239	5)
(240	2)	(241	25)	(242	7)	(243	129)	(244	18)
(245	7)	(246	2)	(247	3)	(248	4)	(249	2)
(250	3)	(253	3)	(254	3)	(257	1)	(258	2)
(259	2)	(260	1)	(261	2)	(263	2)	(264	2)
(265	2)	(266	2)	(267	2)	(268	5)	(269	9)
(270	6)	(271	5)	(272	1)	(273	2)	(274	4)
(275	4)	(277	4)	(279	1)	(280	2)	(281	2)
(283	3)	(284	11)	(285	16)	(286	4)	(287	6)
(293	1)	(294	6)	(297	1)	(298	11)	(299	63)
(300	22)	(301	11)	(302	5)	(304	5)	(305	16)
(306	13)	(307	10)	(308	5)	(309	4)	(310	1)
(311	1)	(313	3)	(314	3)	(315	13)	(316	5)
(317	2)	(318	3)	(319	9)	(320	4)	(321	4)
(322	1)	(323	4)	(324	1)	(325	1)	(326	3)
(327	3)	(328	4)	(331	2)	(332	2)	(338	5)
(339	1)	(340	2)	(341	2)	(342	6)	(343	3)
(345	3)	(346	1)	(349	2)	(350	1)	(352	3)
(353	2)	(355	3)	(357	3)	(358	4)	(359	3)
(360	1)	(361	3)	(365	1)	(367	1)	(368	1)
(369	3)	(372	1)	(373	5)	(374	2)	(375	4)
(376	4)	(377	4)	(378	3)	(379	2)	(380	1)
(381	1)	(382	2)	(383	2)	(384	1)	(385	4)
(386	3)	(387	4)	(388	1)	(389	10)	(390	8)
(391	4)	(393	3)	(395	1)	(396	2)	(397	2)
(398	1)	(399	3)	(400	2)	(401	2)	(404	3)
(405	2)	(406	2)	(407	2)	(411	2)	(412	2)
(415	4)	(416	3)	(417	1)	(421	1)	(422	3)
(423	1)	(424	2)	(427	4)	(428	3)	(430	1)
(432	2)	(434	1)	(438	4)	(439	2)	(444	4)
(445	7)	(446	2)	(448	4)	(449	4)	(450	2)
(452	3)	(453	4)	(454	2)	(457	2)	(458	4)
(460	1)	(461	2)	(462	1)	(463	1)	(464	4)
(465	2)	(466	2)	(467	4)	(468	3)	(469	3)
(472	4)	(473	3)	(476	3)	(477	3)	(480	2)
(481	2)	(482	3)	(486	2)	(487	1)	(488	2)
(491	1)	(492	2)	(493	2)	(494	7)	(495	2)
(497	5)	(498	2)	(500	1)	(502	4)	(503	5)
(504	5)	(505	1)	(506	2)	(507	1)	(510	3)
(511	4)	(514	4)	(515	1)	(517	5)	(518	3)
(519	3)	(521	1)	(522	4)	(523	2)	(524	3)
(526	4)	(527	2)	(529	1)	(530	1)	(534	6)
(537	2)	(538	2)	(541	2)	(543	2)	(544	4)
(545	1)	(547	1)	(548	5)	(552	4)	(554	3)
(555	4)	(556	1)	(561	1)	(562	1)	(563	1)
(564	3)	(565	1)	(566	4)	(567	3)	(570	1)
(572	1)	(574	1)	(575	1)	(579	1)	(582	1)
(583	3)	(596	1)	(597	1)				

NAME:12C_1761.3_1313EC75_[757; 2-Desoxy-pentos-3-ylose dimethoxyamine (2TMS)]
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:176004-10-1
RI:1762
RT: 10.782
NUM PEAKS: 86

(73 1000)	(74 100)	(81 5)	(89 133)	(93 3)
(94 5)	(95 18)	(101 53)	(103 122)	(104 11)
(105 57)	(106 6)	(107 3)	(108 5)	(111 10)
(117 87)	(118 10)	(119 17)	(121 9)	(123 3)
(126 14)	(133 157)	(134 19)	(135 12)	(136 1)
(137 3)	(142 278)	(143 52)	(147 234)	(148 41)
(149 31)	(153 8)	(163 16)	(164 3)	(167 17)
(179 1)	(180 3)	(181 5)	(189 12)	(190 5)
(191 17)	(192 3)	(194 2)	(195 4)	(197 3)
(198 2)	(199 25)	(201 27)	(202 3)	(204 12)
(205 51)	(206 9)	(207 3)	(209 1)	(212 3)
(217 50)	(218 9)	(219 3)	(225 8)	(226 4)
(230 7)	(231 667)	(232 103)	(233 28)	(234 3)
(241 2)	(256 1)	(257 10)	(271 3)	(273 5)
(277 2)	(307 7)	(314 3)	(315 27)	(316 7)
(331 5)	(332 3)	(333 5)	(334 2)	(346 2)
(373 1)	(404 1)	(405 9)	(406 3)	(407 2)
(421 3)				

NAME:12C_1796.4_1313EC75_[646; 3-Deoxyglucitol (5TMS)]
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:180001-10-1
RI:1796
RT: 11.055
NUM PEAKS: 263

(70 11)	(71 11)	(72 24)	(73 1000)	(74 90)
(75 119)	(76 9)	(77 4)	(79 1)	(80 4)
(81 5)	(82 6)	(83 2)	(84 42)	(85 18)
(87 7)	(88 5)	(89 70)	(90 7)	(91 6)
(92 1)	(93 8)	(94 4)	(95 110)	(96 10)
(97 4)	(98 14)	(99 11)	(100 10)	(101 45)
(102 7)	(103 123)	(104 12)	(105 92)	(106 9)
(107 5)	(108 3)	(109 2)	(110 3)	(111 11)
(112 7)	(113 6)	(114 1)	(115 9)	(116 22)
(117 67)	(118 9)	(119 11)	(120 2)	(121 7)
(122 3)	(123 10)	(125 3)	(126 21)	(127 8)
(128 3)	(129 26)	(130 7)	(131 28)	(132 6)
(133 77)	(134 9)	(135 8)	(136 3)	(137 2)
(138 3)	(139 7)	(140 4)	(141 4)	(142 21)
(143 14)	(144 4)	(145 4)	(146 3)	(147 192)
(148 29)	(149 26)	(150 3)	(151 4)	(152 3)
(153 8)	(155 4)	(156 15)	(157 7)	(158 17)
(159 6)	(160 2)	(161 2)	(162 1)	(163 8)
(164 2)	(165 2)	(166 2)	(167 22)	(168 7)
(169 5)	(170 4)	(172 2)	(173 3)	(175 4)
(177 2)	(179 2)	(180 1)	(181 3)	(182 2)
(183 6)	(184 4)	(185 3)	(186 7)	(187 3)
(189 10)	(191 20)	(192 3)	(193 2)	(194 3)
(195 4)	(196 2)	(198 2)	(199 90)	(200 17)
(201 29)	(202 6)	(203 2)	(204 10)	(205 44)
(206 8)	(209 2)	(210 1)	(211 2)	(212 5)
(213 3)	(214 2)	(215 2)	(216 11)	(217 55)
(218 11)	(219 5)	(221 1)	(223 1)	(225 7)

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(226    2) (227    2) (228    5) (229    2) (230    5)
(231  105) (232   17) (233    5) (235    1) (236    1)
(241    1) (242    2) (243    9) (244    2) (245    1)
(248    1) (249    1) (253    1) (254    1) (255    2)
(256    2) (257    7) (261    1) (266    1) (268    1)
(269    3) (270    2) (271    2) (273    5) (274    2)
(275    1) (277    3) (278    2) (285    2) (287    1)
(288    1) (289    1) (290    1) (291    1) (296    1)
(299    2) (300    2) (302    2) (304    1) (305    1)
(306    2) (307   12) (308    4) (309    2) (314    2)
(315   21) (316    6) (317    2) (318    3) (319    1)
(323    1) (327    1) (329    1) (330    1) (331    4)
(332    2) (333    6) (334    2) (335    1) (336    1)
(337    1) (342    1) (344    1) (346    2) (347    1)
(351    2) (352    1) (358    1) (359    1) (361    1)
(365    1) (367    1) (376    1) (381    1) (399    1)
(402    1) (404    2) (405    5) (406    2) (412    1)
(414    1) (420    1) (421    2) (422    1) (424    1)
(425    1) (428    1) (432    1) (439    1) (455    1)
(456    1) (462    1) (465    1) (475    1) (479    1)
(480    1) (495    1) (502    1) (504    1) (510    1)
(516    1) (517    1) (520    1) (523    1) (524    1)
(528    1) (529    2) (531    1) (542    1) (543    1)
(545    1) (547    1) (548    1) (552    1) (560    1)
(566    1) (571    1) (590    1)

NAME:12C_3380.0_1274EC11_Lanosta-8,24-dien-3-beta-ol (1TMS)
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:338001-10-1
RI:3380
RT:19.985
NUM PEAKS:  215
( 70   99) ( 72   17) ( 73 1000) ( 74   97) ( 75  732)
( 76   67) ( 77  169) ( 78   49) ( 79  252) ( 80   28)
( 81  444) ( 82   57) ( 83  204) ( 84   20) ( 87   11)
( 88   10) ( 89   30) ( 90   10) ( 91  261) ( 92   37)
( 93  280) ( 94   37) ( 95  457) ( 96   40) ( 97   66)
( 98   10) (101   17) (103   35) (104   10) (105  295)
(106   41) (107  273) (108   41) (109  538) (110   48)
(111   54) (114    8) (115   59) (116   25) (117  129)
(118   27) (119  293) (120   52) (121  251) (122   49)
(123  179) (124   19) (125   12) (127   19) (128   54)
(129  244) (130   55) (131  184) (132   37) (133  211)
(134   47) (135  237) (136   39) (137   88) (138   15)
(139    7) (141   38) (142   39) (143  124) (144   40)
(145  191) (146   42) (147  212) (148   45) (149  134)
(150   22) (151   31) (152   15) (153   14) (154   16)
(155   38) (156   26) (157  133) (158   38) (159  167)
(160   64) (161  167) (162   37) (163   80) (164   15)
(165   29) (166   14) (167   13) (168   10) (169   36)
(170   17) (171   89) (172   33) (173  129) (174   42)
(175  117) (176   18) (177   45) (178   11) (179   16)
(181   12) (182    8) (183   36) (184   16) (185   72)
(186   24) (187  158) (188   33) (189  139) (190   34)
(191   69) (192   17) (193   20) (197   27) (198   13)
(199   59) (200   21) (201   71) (202   21) (203   55)
(204   20) (205   18) (206    8) (207   64) (208   12)
(209   11) (211   27) (212   15) (213   52) (214   29)
(215   86) (216   21) (217   31) (219   10) (220    7)
(225   28) (226   11) (227   79) (228   20) (229   79)
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(230	18)	(231	14)	(232	4)	(233	6)	(237	6)
(239	14)	(240	8)	(241	136)	(242	33)	(243	36)
(244	12)	(245	10)	(253	15)	(254	8)	(255	57)
(256	17)	(257	34)	(258	11)	(259	9)	(265	10)
(266	9)	(267	18)	(269	25)	(270	12)	(271	17)
(272	22)	(273	11)	(281	29)	(282	11)	(283	27)
(284	7)	(285	11)	(286	5)	(295	9)	(297	16)
(298	8)	(299	6)	(309	15)	(310	6)	(311	27)
(312	11)	(317	5)	(319	6)	(323	15)	(325	10)
(328	6)	(331	9)	(332	6)	(335	4)	(349	5)
(350	11)	(351	15)	(352	9)	(386	8)	(389	3)
(393	276)	(394	162)	(395	38)	(408	4)	(413	10)
(427	4)	(450	6)	(477	4)	(482	11)	(483	70)
(484	72)	(485	27)	(486	9)	(487	5)	(497	14)
(498	77)	(499	67)	(500	28)	(501	10)	(506	6)

NAME:12C_3081.9_1160EC23_[808; Adenosine-5´-monophosphate (5TMS)]
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:308001-10-1
RI:3082
RT:18.685
NUM PEAKS: 174

(70	5)	(71	5)	(72	18)	(73	1000)	(74	93)
(75	110)	(76	7)	(77	11)	(80	3)	(81	29)
(82	3)	(85	8)	(86	4)	(87	5)	(89	7)
(92	3)	(93	3)	(94	5)	(95	7)	(97	12)
(98	4)	(99	14)	(100	3)	(101	27)	(102	6)
(103	12)	(105	4)	(107	3)	(108	29)	(109	5)
(111	8)	(113	18)	(114	3)	(115	18)	(116	11)
(117	11)	(118	3)	(119	14)	(120	3)	(121	6)
(125	9)	(126	3)	(127	11)	(129	66)	(130	9)
(131	20)	(132	5)	(133	78)	(134	12)	(135	85)
(136	80)	(137	12)	(139	3)	(140	24)	(141	15)
(142	18)	(143	26)	(144	4)	(145	7)	(146	3)
(147	143)	(148	30)	(149	24)	(150	6)	(151	9)
(153	12)	(154	3)	(155	5)	(156	3)	(157	6)
(158	3)	(159	4)	(160	3)	(161	4)	(162	3)
(163	3)	(164	40)	(165	8)	(167	6)	(168	3)
(169	469)	(170	67)	(171	44)	(172	6)	(173	4)
(174	4)	(175	4)	(177	3)	(178	3)	(179	4)
(181	12)	(183	6)	(184	5)	(185	4)	(186	7)
(187	3)	(189	4)	(190	3)	(191	6)	(193	10)
(194	5)	(195	14)	(196	3)	(197	5)	(204	3)
(205	3)	(206	20)	(207	27)	(208	31)	(209	8)
(210	4)	(211	83)	(212	13)	(213	8)	(214	10)
(215	16)	(216	5)	(217	18)	(218	5)	(221	3)
(225	18)	(226	3)	(227	17)	(228	4)	(229	4)
(230	125)	(231	29)	(232	12)	(233	3)	(234	16)
(235	4)	(241	3)	(243	67)	(244	15)	(245	9)
(248	3)	(249	4)	(250	16)	(251	3)	(253	4)
(257	6)	(258	69)	(259	20)	(260	8)	(262	7)
(265	22)	(266	7)	(283	3)	(285	7)	(298	3)
(299	74)	(300	23)	(301	12)	(302	5)	(303	6)
(304	13)	(305	3)	(306	8)	(307	3)	(314	8)
(315	240)	(316	64)	(317	33)	(318	6)	(371	9)
(372	3)	(382	21)	(383	9)	(384	4)	(387	4)
(394	20)	(395	8)	(396	3)	(411	3)		

NAME:12C_2679.2_1160EC23_[837; alpha-D-Fructofuranose-1,6-bisphosphate (7TMS)]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:268001-10-1
RI:2679
RT:16.787
NUM PEAKS: 170

(71 4)	(72 15)	(73 1000)	(74 88)	(75 110)
(76 6)	(77 9)	(81 8)	(82 21)	(83 7)
(85 5)	(86 3)	(87 4)	(89 5)	(96 13)
(97 7)	(98 4)	(99 6)	(100 3)	(101 15)
(102 6)	(103 33)	(104 4)	(105 3)	(109 8)
(111 5)	(113 12)	(115 8)	(116 5)	(117 21)
(118 3)	(119 6)	(125 5)	(127 6)	(128 3)
(129 86)	(130 14)	(131 20)	(133 53)	(134 7)
(135 13)	(137 4)	(140 13)	(141 17)	(142 11)
(143 24)	(144 6)	(145 5)	(146 3)	(147 199)
(148 32)	(149 29)	(150 3)	(151 9)	(153 3)
(155 9)	(156 8)	(157 17)	(158 4)	(159 3)
(163 3)	(167 3)	(169 12)	(177 9)	(181 7)
(182 3)	(183 11)	(184 4)	(187 3)	(189 10)
(190 7)	(191 37)	(192 6)	(193 10)	(195 10)
(196 5)	(197 4)	(199 3)	(200 14)	(201 4)
(202 3)	(203 3)	(204 37)	(205 17)	(206 5)
(207 25)	(208 5)	(209 5)	(210 3)	(211 49)
(212 8)	(213 6)	(214 11)	(215 57)	(216 14)
(217 63)	(218 14)	(219 8)	(221 33)	(222 9)
(223 5)	(225 29)	(226 6)	(227 16)	(228 3)
(229 9)	(230 68)	(231 23)	(232 7)	(241 6)
(243 10)	(244 3)	(255 5)	(257 36)	(258 9)
(259 5)	(269 3)	(270 4)	(271 15)	(272 4)
(273 3)	(281 7)	(283 8)	(284 3)	(285 9)
(295 10)	(296 3)	(297 3)	(298 7)	(299 124)
(300 34)	(301 18)	(302 3)	(303 7)	(305 3)
(313 5)	(314 7)	(315 166)	(316 46)	(317 24)
(318 5)	(319 7)	(328 22)	(329 7)	(330 3)
(341 3)	(343 6)	(345 4)	(347 6)	(348 3)
(355 3)	(356 4)	(357 10)	(358 3)	(361 3)
(369 7)	(370 3)	(371 3)	(373 7)	(387 17)
(388 7)	(389 4)	(423 3)	(436 3)	(444 5)
(445 24)	(446 11)	(447 6)	(513 3)	(589 6)

NAME:12C_2339.5_1160EC23_[882; Pseudouridine (5TMS)]
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:234001-10-1
RI:2340
RT:14.991
NUM PEAKS: 133

(70 4)	(72 16)	(73 1000)	(74 79)	(75 31)
(82 3)	(86 4)	(89 8)	(98 1)	(99 6)
(100 30)	(101 13)	(103 86)	(104 6)	(105 3)
(106 5)	(111 5)	(113 6)	(115 2)	(116 3)
(117 12)	(119 4)	(122 1)	(125 5)	(126 1)
(127 17)	(128 1)	(129 35)	(130 3)	(131 24)
(132 3)	(133 47)	(134 5)	(135 2)	(136 1)
(140 3)	(141 2)	(142 7)	(143 30)	(144 5)
(145 3)	(147 159)	(148 24)	(149 17)	(151 2)
(154 3)	(157 6)	(158 6)	(159 1)	(166 2)
(172 2)	(177 2)	(179 1)	(180 1)	(184 1)
(185 2)	(186 2)	(189 13)	(191 7)	(192 3)
(193 2)	(198 2)	(201 2)	(202 5)	(203 3)
(204 5)	(207 2)	(209 2)	(211 1)	(215 26)

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(216    7) (217  498) (218   97) (219   44) (220    4)
(221    2) (225    2) (229    1) (230   18) (231    3)
(239    4) (252    1) (253    5) (254    2) (255    4)
(257    3) (265    2) (266    1) (267   10) (268    2)
(269   25) (270    6) (281    4) (282    2) (283    7)
(285    1) (327    2) (329    1) (355   13) (356    9)
(357   64) (358   22) (359   10) (369    3) (370    3)
(371    9) (372    5) (373    2) (382    2) (383    9)
(384    5) (385    2) (386    4) (409    2) (410    1)
(411   10) (412    5) (423    5) (424   32) (425   18)
(426    8) (443    1) (496    6) (497    5) (498    2)
(499    3) (500    2) (501    2) (513    1) (514    3)
(589    5) (590    2) (591    2)

NAME:12C_2651.1_1160EC15_[721; Adenosine (4TMS)]
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:265001-10-1
RI:2651
RT:16.639
NUM PEAKS:  46
( 73 1000) ( 74   67) ( 76    6) ( 79   15) (101   15)
(103  102) (110   12) (116    5) (129   17) (133   46)
(143   28) (147  115) (148    6) (157   10) (169   19)
(186    5) (192   76) (202    5) (204   21) (206   22)
(208   59) (217  134) (218   35) (230  199) (231   35)
(236  182) (237   39) (243   34) (245   92) (246   19)
(259   14) (266   24) (279   12) (287    6) (322   28)
(335   15) (374    3) (375    7) (385    8) (463    8)
(475   16) (495    5) (502    5) (519    9) (524    6)
(540    8)

NAME:12C_1924.2_1313EC57_Mannitol (6TMS)
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:193002-10-1
RI:1924
RT:12.009
NUM PEAKS:  126
( 70    2) ( 72   14) ( 73 1000) ( 74   88) ( 75   45)
( 83   11) ( 87    6) ( 88    5) ( 89   31) ( 90    3)
( 97    9) ( 99    4) (101   25) (102    4) (103  188)
(104   16) (111    2) (113    4) (115    4) (116    5)
(117  120) (118   11) (119    9) (127    2) (129   93)
(130   10) (131   32) (132    3) (133   60) (134    8)
(135    5) (141    2) (142    1) (143   13) (144    2)
(145    4) (147  324) (148   49) (149   26) (150    3)
(151    2) (157   64) (158    8) (159    4) (161    3)
(163    3) (169    6) (170    1) (175    5) (177    2)
(183    6) (186    1) (189   43) (190   10) (191   42)
(192    6) (193    2) (203    4) (204   46) (205  167)
(206   32) (207   13) (215    1) (216    2) (217  167)
(218   34) (219   15) (220    1) (221    5) (222    1)
(229   17) (230    6) (231   17) (232    4) (233    1)
(239    1) (246    1) (249    1) (250    1) (252    1)
(255    7) (256    2) (257    1) (259    6) (260    1)
(277    6) (278    3) (279    1) (291    6) (292    3)
(293    1) (305    7) (306    5) (307   21) (308    7)
(309    2) (318    9) (319  140) (320   47) (321   20)
(322    4) (323    1) (329    1) (330    2) (331   16)
(332    6) (333    2) (334    1) (345    5) (346    2)
(397    1) (409    1) (419    2) (420    2) (421    4)
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(422 1) (423 1) (424 1) (433 1) (477 1)
(485 1) (525 1) (526 1) (529 1) (552 1)
(579 1)

NAME:12C_1920.1_1313EC57_[529; Methylcitric acid (4TMS)]
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:192007-10-1
RI:1920
RT:11.983
NUM PEAKS: 157
(72 34) (73 1000) (74 107) (75 160) (76 8)
(77 7) (80 2) (81 13) (83 4) (89 11)
(90 3) (91 5) (92 2) (97 16) (99 8)
(101 15) (104 7) (105 11) (109 8) (116 16)
(118 7) (119 7) (122 2) (125 35) (127 6)
(129 29) (131 41) (133 77) (134 11) (135 10)
(136 3) (141 3) (143 12) (144 5) (145 4)
(147 314) (148 50) (149 53) (150 6) (151 3)
(152 2) (153 11) (155 22) (159 2) (161 3)
(163 3) (169 12) (170 3) (171 16) (173 7)
(181 5) (183 3) (185 3) (189 13) (190 6)
(192 3) (193 2) (197 30) (198 4) (199 9)
(203 6) (204 29) (207 7) (208 2) (209 3)
(210 2) (215 4) (216 3) (218 18) (219 6)
(221 19) (222 3) (225 5) (226 2) (227 3)
(242 3) (243 50) (244 12) (245 11) (246 2)
(247 1) (248 1) (249 2) (251 1) (252 2)
(259 4) (271 7) (273 2) (278 2) (286 3)
(287 106) (288 27) (289 11) (290 3) (291 3)
(292 2) (293 2) (299 6) (300 1) (301 2)
(305 4) (310 1) (314 1) (315 1) (325 3)
(332 3) (333 3) (334 3) (335 1) (336 2)
(337 1) (345 1) (347 3) (359 1) (360 4)
(361 20) (362 6) (376 2) (377 10) (378 3)
(386 2) (387 1) (388 1) (389 5) (403 1)
(404 1) (408 1) (409 1) (410 1) (411 1)
(414 2) (424 1) (429 1) (430 1) (439 2)
(443 1) (449 1) (453 1) (456 1) (461 3)
(477 1) (478 4) (479 7) (480 4) (481 3)
(482 1) (485 1) (493 2) (496 2) (497 2)
(508 1) (510 1) (526 2) (529 1) (547 1)
(555 1) (558 1)

NAME:12C_1544.5_1313EC75_Erythronic acid (4TMS)
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:154001-10-1
RI:1545
RT:9.099
NUM PEAKS: 72
(70 335) (71 4) (72 13) (73 1000) (74 78)
(83 10) (89 22) (99 5) (101 12) (102 92)
(103 103) (104 12) (112 122) (113 11) (117 148)
(118 12) (119 13) (129 35) (130 74) (131 35)
(132 8) (133 70) (134 8) (135 6) (136 2)
(139 2) (143 33) (144 9) (147 485) (148 79)
(149 44) (150 5) (152 3) (163 5) (167 2)
(177 17) (178 4) (180 6) (181 3) (185 3)
(189 22) (190 3) (196 1) (203 7) (204 18)
(205 100) (206 18) (214 35) (215 2) (217 84)
(218 16) (219 12) (220 121) (229 10) (239 6)

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(241    7) (242    2) (254   26) (255    5) (256    2)
(269    3) (291   19) (292  138) (293   41) (294   17)
(305    2) (319    8) (320    2) (321    2) (379    2)
(409    3) (535    1)

NAME:12C_1291.0_1185EK01_Leucine (2TMS)
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:129002-01-1
RI:1291
NUM PEAKS:  98
( 70   21) ( 71   10) ( 72   27) ( 73 1000) ( 74  112)
( 75  178) ( 76   14) ( 77   55) ( 78    5) ( 79    8)
( 80    2) ( 81    1) ( 82    4) ( 83    3) ( 84   13)
( 85    7) ( 86   46) ( 87   10) ( 88    4) ( 89    4)
( 90    1) ( 91    1) ( 92    2) ( 93    1) ( 94    1)
( 95    1) ( 96    5) ( 97    3) ( 98    6) ( 99   10)
(100   89) (101   17) (102  168) (103   44) (104    9)
(105    5) (110    1) (111    1) (112    3) (113    2)
(114    4) (115   25) (116   32) (117   25) (118    5)
(119    5) (126    2) (127    1) (128   23) (129    9)
(130   41) (131   19) (132   20) (133   41) (134    7)
(135    3) (140    1) (142   14) (143    4) (144    5)
(145    1) (146    4) (147  117) (148   19) (149   10)
(150    1) (156    3) (157    2) (158  720) (159  105)
(160   32) (161    3) (163    1) (170    8) (171    2)
(172    1) (174    3) (175    2) (176    2) (177    2)
(186    1) (188    1) (191    1) (202    1) (203    3)
(204    2) (205    4) (206    1) (207    1) (218   21)
(219    5) (220    2) (231    1) (232   25) (233    6)
(234    2) (260    7) (261    2)

NAME:12C_1273.1_1313EC43_[938; Sulfuric acid (2TMS)]
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:127005-10-1
RI:1273
RT:6.066
NUM PEAKS:  344
( 72   37) ( 73  278) ( 74   26) ( 76   10) ( 83    5)
( 84   13) ( 88    7) ( 89   23) ( 90    7) ( 94    4)
( 95   11) ( 98    7) (107   12) (108    9) (109    7)
(111    6) (112    6) (113    5) (114   15) (115   17)
(116   16) (118   12) (119   13) (120    9) (122    9)
(123   18) (125   12) (128    6) (130    4) (132   30)
(133   33) (134   18) (137    5) (138   10) (139   28)
(140    8) (141   10) (143    7) (144    4) (145    9)
(147 1000) (148  179) (149  106) (150   17) (151    7)
(152    7) (153    6) (154    8) (155    4) (156    6)
(158    7) (159    9) (160    6) (162   10) (164    4)
(165    5) (168    9) (169    7) (170    6) (171    6)
(172    5) (173    5) (177    6) (181    7) (182    8)
(184    7) (185    5) (186    9) (187    7) (188    7)
(189    6) (190    6) (191    7) (193    3) (194    4)
(197    8) (198    7) (201    5) (202    6) (205    8)
(206    3) (208    6) (209    6) (210    6) (211    8)
(216    6) (217    8) (218    6) (222    5) (223    6)
(224    4) (226    7) (227  187) (228   32) (229   28)
(230   11) (233    4) (234    2) (235    5) (236    8)
(237    7) (238    6) (239    6) (240    7) (241    6)
(242    7) (243    8) (244    6) (245    8) (247    8)
(249    6) (250    6) (252    8) (253    7) (254    9)
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(255 8) (256 8) (257 4) (258 8) (262 7)
(263 7) (264 4) (265 8) (267 9) (270 8)
(271 9) (272 9) (275 9) (277 11) (279 12)
(280 12) (281 9) (282 10) (283 8) (284 7)
(288 9) (289 7) (292 7) (293 8) (296 5)
(297 8) (300 9) (301 6) (302 10) (303 3)
(306 4) (308 3) (309 4) (310 5) (311 4)
(313 5) (314 4) (316 8) (317 6) (319 5)
(320 4) (322 7) (325 6) (326 9) (327 6)
(328 10) (329 8) (330 9) (331 7) (332 7)
(333 8) (334 5) (335 6) (336 6) (338 5)
(341 6) (342 7) (345 6) (346 7) (347 8)
(348 7) (349 7) (350 6) (351 9) (352 6)
(353 9) (354 12) (355 6) (356 9) (358 11)
(360 4) (361 7) (362 8) (363 13) (369 12)
(373 8) (374 8) (375 15) (376 8) (381 9)
(382 7) (383 7) (384 11) (385 10) (386 12)
(388 10) (389 12) (393 6) (394 6) (395 9)
(396 16) (398 7) (400 11) (401 10) (402 9)
(403 8) (406 8) (407 9) (408 8) (409 7)
(410 7) (411 4) (415 7) (416 8) (417 8)
(418 7) (419 5) (420 7) (421 6) (422 7)
(423 4) (424 6) (425 10) (426 4) (428 5)
(429 7) (430 10) (431 8) (432 4) (433 4)
(435 5) (436 7) (439 6) (440 6) (441 10)
(442 7) (443 5) (444 5) (445 7) (446 6)
(449 8) (452 9) (453 10) (454 8) (457 4)
(458 7) (459 10) (460 11) (462 8) (463 10)
(465 10) (466 12) (467 7) (468 9) (469 8)
(470 11) (471 8) (472 6) (474 8) (475 6)
(476 7) (477 10) (478 9) (479 6) (481 9)
(482 11) (483 5) (484 6) (485 8) (486 14)
(487 9) (488 7) (489 5) (492 8) (494 10)
(495 7) (496 11) (498 8) (499 11) (500 11)
(502 11) (503 10) (505 6) (506 12) (509 4)
(510 6) (511 6) (512 8) (513 8) (514 5)
(516 7) (517 12) (518 8) (519 5) (521 7)
(522 9) (523 5) (524 7) (525 5) (526 9)
(528 9) (529 12) (530 6) (531 7) (532 7)
(533 7) (534 7) (535 9) (536 4) (537 11)
(538 8) (539 4) (541 7) (545 6) (546 4)
(548 9) (549 8) (551 5) (552 7) (553 2)
(555 5) (556 3) (557 4) (558 7) (559 4)
(561 6) (563 3) (564 4) (565 4) (567 3)
(570 5) (572 6) (573 4) (578 4) (579 4)
(580 3) (583 3) (589 5) (595 2)

NAME:12C_1269.8_1135EC44_Urea (2TMS)
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:127002-01-1
RI:1270
RT:402.296
RSN:2975.0
NUM PEAKS: 51
(70 62) (71 56) (72 79) (73 377) (74 147)
(75 115) (76 11) (77 6) (78 21) (79 64)
(80 5) (84 10) (85 24) (86 21) (87 78)
(88 10) (90 6) (99 136) (100 100) (101 33)
(102 20) (103 12) (105 8) (111 5) (113 15)
(114 15) (115 31) (116 12) (117 6) (130 68)

(131 67) (132 56) (133 31) (134 6) (146 66)
(147 1000) (148 161) (149 78) (150 7) (155 4)
(157 15) (171 158) (172 29) (173 65) (174 11)
(175 4) (186 9) (189 434) (190 79) (191 35)
(204 21)

NAME:12C_1723.7_1160EC15_2-Aminoadipic acid (3TMS)
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:172006-10-1
RI:1724
RT:10.996
NUM PEAKS: 183
(70 20) (71 15) (72 35) (73 1000) (74 100)
(75 283) (76 21) (77 23) (78 5) (79 9)
(80 12) (81 8) (82 6) (83 11) (85 28)
(86 15) (87 9) (88 5) (89 6) (91 2)
(92 1) (93 15) (94 2) (95 9) (96 8)
(97 20) (98 47) (99 17) (100 135) (101 24)
(102 12) (104 5) (107 2) (108 10) (109 3)
(110 3) (111 9) (112 9) (113 4) (114 13)
(115 86) (116 30) (117 29) (118 5) (119 7)
(121 1) (122 1) (123 4) (124 2) (125 2)
(126 5) (127 4) (128 219) (129 199) (130 36)
(131 53) (132 23) (133 58) (134 9) (135 6)
(136 1) (137 3) (138 3) (141 2) (142 8)
(143 7) (144 2) (145 6) (146 3) (147 178)
(148 31) (149 39) (150 6) (151 14) (152 4)
(153 4) (154 33) (159 3) (161 2) (162 1)
(163 12) (164 3) (165 1) (168 3) (169 1)
(170 37) (171 6) (172 13) (174 10) (175 2)
(182 13) (183 3) (187 1) (188 11) (193 2)
(198 1) (200 2) (202 8) (203 18) (208 1)
(213 2) (216 4) (217 304) (218 87) (219 34)
(220 5) (221 6) (228 8) (231 1) (232 2)
(233 2) (234 1) (235 1) (242 2) (243 11)
(244 71) (245 18) (246 8) (250 1) (251 1)
(252 1) (254 2) (256 1) (259 3) (260 357)
(261 83) (262 33) (263 5) (266 1) (272 28)
(273 6) (274 3) (278 1) (286 1) (287 1)
(288 6) (289 2) (290 1) (291 7) (292 2)
(293 2) (294 1) (301 2) (302 2) (313 1)
(317 1) (318 1) (326 1) (334 3) (335 2)
(337 1) (342 1) (348 1) (361 1) (362 15)
(363 6) (364 3) (376 1) (377 9) (378 4)
(379 1) (391 1) (393 1) (417 1) (418 2)
(428 1) (438 1) (450 1) (465 1) (472 1)
(478 1) (486 1) (497 1) (503 1) (513 1)
(523 1) (529 1) (532 1) (537 1) (540 1)
(541 1) (547 1) (562 1)

NAME:12C_1739.1_1274EC11_Aspartic acid (4TMS)
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:174003-10-1
RI:1739
RT:11.121
NUM PEAKS: 117
(70 40) (71 24) (72 30) (73 1000) (74 102)
(79 20) (80 14) (88 6) (89 30) (92 5)
(94 9) (96 9) (98 9) (99 46) (100 58)
(105 24) (106 9) (107 5) (108 4) (113 7)

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(114   10) (121    4) (124    5) (127   21) (130   26)
(131   23) (133   89) (134   11) (135    5) (141   13)
(142    8) (143   22) (144    6) (145    4) (146   13)
(149   25) (150   10) (157   22) (158   19) (159   36)
(160   11) (161    8) (162    3) (163   83) (164   17)
(169   12) (171   16) (172   75) (173   25) (177    7)
(183   10) (185   18) (188    6) (191   26) (197    4)
(199   10) (202   33) (205  243) (206   45) (207   23)
(213    6) (215   34) (216   13) (221   26) (222    9)
(223    7) (242    4) (244    8) (246    6) (247    6)
(257    5) (259    6) (262    5) (264    4) (273   26)
(275    9) (276    5) (279   21) (280    9) (287   12)
(288   21) (289   22) (290   24) (291    8) (299    8)
(302    5) (304   31) (306    7) (316    5) (317    7)
(330    7) (331   13) (332    6) (347    8) (363   14)
(364    7) (365    5) (378    8) (379    5) (380    6)
(382    3) (406   14) (407   10) (421    3) (422    5)
(424    7) (430    5) (432    5) (454    6) (498    7)
(506    4) (511    5) (519    4) (527    4) (529    4)
(553    4) (565    4)
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NAME:12C_2225.6_1178EC20_Tryptophan (3TMS)
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:223001-10-1
RI:2226
RT:14.362
NUM PEAKS:  95
( 72   12) ( 73 1000) ( 76    6) ( 77   12) ( 91    3)
( 92    3) ( 94    3) ( 96   25) (100   13) (103    3)
(105    8) (106    3) (110    8) (116   15) (122    3)
(124    3) (128    7) (129   32) (130   19) (131   41)
(132   42) (133   21) (134    8) (138    3) (142    3)
(145   48) (146   17) (147   29) (148    5) (152    7)
(155    3) (156    9) (159    9) (160    8) (161    6)
(170    3) (173    5) (175    3) (180    8) (184    6)
(187   12) (188    8) (189    7) (190    8) (200   11)
(201    5) (202  705) (203  155) (204   45) (215    8)
(218   17) (219   30) (220   10) (221    5) (222    5)
(229    3) (230    8) (231    7) (232    3) (233    4)
(235    7) (236    3) (246    3) (248    3) (257    3)
(261    4) (264    6) (265    6) (291   38) (292   15)
(293    6) (303    4) (327    4) (337    4) (338    4)
(351    4) (367    3) (379    3) (394    3) (406    4)
(407    8) (408    9) (409    3) (421    3) (422   10)
(423    8) (424    4) (425    3) (427    3) (437    4)
(446    3) (462    5) (496    3) (542    3) (564    3)
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NAME:12C_2770.4_1160EC15_[626; 5'-Methylthioadenosine (3TMS)]
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:277004-10-1
RI:2770
RT:17.269
NUM PEAKS:  24
( 73 1000) ( 74  105) ( 87   43) (101   75) (108   46)
(115   35) (116   53) (119   32) (127   34) (135   63)
(136  276) (137   30) (148   36) (164  692) (165   43)
(169  261) (175  769) (176   98) (177   35) (188  441)
(190   35) (208   45) (234   13) (426   28)
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NAME:12C_1324.1_1313EC07_Nicotinic acid (1TMS)
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COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:133004-10-1
RI:1324
RT:6.689
NUM PEAKS: 17
(78 769) (79 88) (83 111) (106 622) (107 47)
(110 11) (111 38) (112 48) (136 836) (137 90)
(138 26) (141 49) (180 1000) (181 149) (182 36)
(186 61) (195 41)

NAME:12C_2427.5_1313EC07_[931; myo-Inositol-1-phosphate (7TMS)]
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:243001-10-1
RI:2428
RT:14.977
NUM PEAKS: 283
(70 3) (71 3) (72 16) (73 1000) (74 89)
(75 76) (76 4) (77 10) (78 1) (79 3)
(80 1) (81 14) (82 2) (83 4) (84 1)
(85 5) (86 2) (87 6) (88 2) (89 5)
(90 1) (91 3) (92 1) (93 2) (94 1)
(95 2) (96 2) (97 2) (98 2) (99 5)
(100 1) (101 8) (102 4) (103 25) (105 6)
(106 2) (107 3) (108 1) (109 5) (110 1)
(111 6) (112 1) (113 5) (114 1) (115 7)
(116 5) (117 7) (118 1) (119 6) (120 1)
(121 3) (123 1) (125 2) (126 1) (127 6)
(128 1) (129 36) (130 4) (131 21) (132 4)
(133 64) (134 9) (135 13) (136 2) (137 6)
(138 1) (139 2) (140 1) (141 3) (142 3)
(143 18) (144 2) (145 3) (146 1) (147 252)
(148 41) (149 26) (150 3) (151 6) (152 1)
(153 5) (154 2) (155 5) (156 4) (157 5)
(158 1) (159 2) (160 1) (161 3) (162 1)
(163 3) (164 1) (165 2) (166 1) (167 2)
(168 1) (169 5) (170 1) (171 1) (173 1)
(175 3) (176 1) (177 3) (178 1) (179 2)
(180 1) (181 8) (182 2) (183 4) (184 1)
(185 1) (187 1) (189 8) (190 7) (191 47)
(192 9) (193 12) (194 2) (195 4) (196 1)
(197 2) (199 1) (201 2) (202 1) (203 2)
(204 15) (205 7) (206 2) (207 15) (208 4)
(209 3) (210 2) (211 35) (212 6) (213 4)
(214 1) (215 4) (216 2) (217 46) (218 10)
(219 4) (221 8) (222 2) (223 1) (224 1)
(225 9) (226 2) (227 11) (228 3) (229 2)
(230 11) (231 4) (232 1) (233 1) (235 1)
(237 1) (239 2) (240 1) (241 2) (242 1)
(243 11) (244 3) (245 3) (246 9) (247 2)
(248 1) (249 1) (251 1) (252 1) (253 1)
(254 1) (255 8) (256 2) (257 3) (258 1)
(259 1) (265 3) (266 1) (267 1) (268 1)
(269 3) (270 2) (271 3) (272 1) (273 1)
(278 1) (283 4) (284 2) (285 7) (286 2)
(287 1) (291 5) (292 2) (293 1) (297 1)
(298 12) (299 108) (300 32) (301 17) (302 3)
(303 1) (304 2) (305 8) (306 4) (307 2)
(308 1) (312 1) (313 4) (314 11) (315 89)
(316 26) (317 25) (318 104) (319 35) (320 15)
(321 3) (322 1) (327 1) (328 1) (329 1)

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(330    1) (331    2) (332    1) (333    1) (340    1)
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(346    2) (347    1) (357    1) (358    1) (359    1)
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(371    1) (372    2) (373    6) (374    3) (375    1)
(385    2) (386   11) (387   39) (388   19) (389   19)
(390    6) (391    3) (392    1) (417    1) (418    1)
(419    2) (420    1) (421    1) (428    1) (429    3)
(430    1) (431    2) (432    5) (433    4) (434    2)
(435    1) (441    1) (442    1) (443    1) (444    1)
(455    1) (456    1) (457    1) (458    1) (459    1)
(460    1) (461    1) (462    1) (469    1) (470    2)
(471    1) (472    1) (507    1)

NAME:12C_2000.0_1313EC07_Panthotenic acid (3TMS)
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:200006-10-1
RI:2000
RT:12.490
NUM PEAKS:  107
( 78  209) ( 79  192) ( 80   14) (108   92) (109   16)
(123   74) (124  132) (127   69) (128   70) (129  254)
(143   25) (157 1000) (166   33) (170   38) (182    1)
(184   30) (185   15) (197    4) (198   16) (201  777)
(202   71) (247  119) (274    8) (284    7) (285   26)
(286    9) (290   82) (291  871) (292  113) (330   17)
(346   72) (347   28) (359   43) (360    3) (361   18)
(374   21) (375   21) (386   18) (390   14) (391   15)
(406   68) (420  168) (421   85) (433    7) (434   44)
(445   66) (446   27) (448   20) (449    1) (450    5)
(463   50) (465   16) (467    4) (468    5) (475    3)
(480   18) (481   13) (482   53) (487   55) (493   34)
(494   12) (496   29) (497   17) (502    9) (505   28)
(506   19) (510    5) (511   55) (514   35) (515   15)
(516    7) (519   67) (522   73) (523   12) (524   49)
(525    1) (526    3) (534   60) (539   64) (540   13)
(543   76) (545    5) (547   57) (548   15) (549   20)
(551   20) (552   68) (553    1) (557   14) (562    4)
(563    6) (569    8) (570   37) (575    6) (577   26)
(579   13) (580   16) (582   12) (583   25) (585   13)
(586   14) (588   28) (591   12) (593   12) (595   10)
(596   14) (597    2)

NAME:12C_1292.9_1313EC11_Leucine (2TMS)
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:129002-10-1
RI:1293
RT:6.287
NUM PEAKS:  4
( 79   83) (158 1000) (159   20) (232    2)

NAME:12C_1490.1_2119DC04_[545; 2,3-Dimethylsuccinic acid (2TMS)]
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:149003-10-1
RI:1490
RT:20.245
NUM PEAKS:  166
( 41  217) ( 42   21) ( 43  227) ( 44   61) ( 45  122)
( 47   52) ( 50   20) ( 52   23) ( 53   34) ( 54   11)
( 57   15) ( 58   41) ( 59  316) ( 60   26) ( 61   65)
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(62 6) (63 11) (65 17) (66 6) (67 79)
(68 21) (69 185) (70 11) (71 52) (72 11)
(73 408) (74 32) (75 1000) (76 82) (77 49)
(79 35) (81 30) (82 19) (83 116) (84 6)
(85 123) (86 13) (89 734) (90 61) (91 64)
(92 7) (93 8) (95 128) (96 18) (97 46)
(98 10) (99 55) (103 19) (105 44) (107 8)
(108 2) (110 4) (111 9) (113 267) (114 22)
(119 9) (120 4) (123 15) (125 17) (127 72)
(131 84) (132 11) (137 7) (139 2) (141 20)
(143 479) (144 55) (145 114) (146 42) (147 826)
(148 134) (149 30) (154 5) (155 79) (156 11)
(157 278) (158 38) (159 237) (160 27) (161 85)
(162 24) (163 355) (164 53) (165 34) (166 7)
(169 8) (170 18) (173 41) (174 13) (179 3)
(180 6) (185 31) (186 8) (187 44) (191 310)
(192 43) (193 30) (196 4) (197 3) (201 59)
(207 435) (208 64) (209 47) (210 7) (212 2)
(213 5) (215 14) (216 7) (217 12) (226 3)
(229 72) (231 184) (232 33) (239 2) (244 2)
(247 174) (248 36) (249 20) (250 5) (254 5)
(258 3) (259 28) (261 24) (262 3) (270 3)
(271 3) (275 362) (276 92) (277 35) (278 5)
(291 87) (292 21) (293 7) (299 4) (301 2)
(313 3) (319 46) (320 10) (321 2) (322 2)
(333 3) (346 2) (354 2) (356 2) (371 2)
(380 3) (388 2) (397 2) (407 3) (434 2)
(439 3) (453 2) (466 3) (476 2) (479 3)
(515 2) (521 2) (527 2) (533 2) (552 2)
(562 3) (567 2) (579 2) (594 2) (596 5)
(598 7)

NAME:12C_2816.0_2119DC04_[542; Maltose methoxyamine [BP] (8TMS); alpha-D-Glc-(1,4)-alpha-D-Glc]
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:282003-10-1
RI:2816
RT:41.182
NUM PEAKS: 75
(44 171) (48 62) (64 42) (73 1000) (82 73)
(88 62) (103 130) (104 92) (108 67) (111 127)
(129 273) (130 78) (133 147) (143 44) (147 245)
(152 34) (167 53) (169 195) (172 33) (175 40)
(179 127) (181 52) (191 520) (192 167) (197 50)
(202 43) (207 109) (214 26) (215 29) (217 105)
(218 44) (220 30) (229 57) (236 29) (241 39)
(242 28) (243 110) (244 76) (246 29) (251 35)
(252 59) (267 42) (270 47) (275 32) (281 53)
(319 64) (321 44) (323 32) (333 45) (353 24)
(357 55) (361 166) (362 69) (363 56) (386 29)
(393 25) (400 22) (407 40) (431 37) (439 27)
(443 24) (457 24) (464 36) (469 41) (488 29)
(506 37) (507 25) (509 37) (521 27) (523 25)
(530 33) (550 24) (581 26) (587 26) (597 24)

NAME:12C_1685.1_1313EC57_Ribose methoxyamine (4TMS)
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer |RI:1685 |RI:1685 |RI:1685
CASNO:168002-10-1
RI:1685
RT:10.186

SOURCE:C:\NISTMS\AMDIS32\LIB\MS_RI.msp
NUM PEAKS: 431

(70 75)	(71 28)	(73 1000)	(74 24)	(78 10)
(82 16)	(83 39)	(84 24)	(85 16)	(86 7)
(87 13)	(88 10)	(89 66)	(90 11)	(91 28)
(92 6)	(95 5)	(96 4)	(97 4)	(98 8)
(99 17)	(101 33)	(102 5)	(103 282)	(104 31)
(105 37)	(106 6)	(107 4)	(108 2)	(109 21)
(111 5)	(112 10)	(113 17)	(117 59)	(119 18)
(120 5)	(121 5)	(122 4)	(123 4)	(126 9)
(127 8)	(128 18)	(129 43)	(133 69)	(135 8)
(136 2)	(137 6)	(138 5)	(139 5)	(140 15)
(143 6)	(144 40)	(145 19)	(147 244)	(148 42)
(149 17)	(151 6)	(152 4)	(153 4)	(155 55)
(156 12)	(157 8)	(158 10)	(160 127)	(161 23)
(162 11)	(163 11)	(164 6)	(165 4)	(166 3)
(167 7)	(168 6)	(170 7)	(171 4)	(172 7)
(173 27)	(174 19)	(175 12)	(176 5)	(177 6)
(178 5)	(179 3)	(181 5)	(182 7)	(183 5)
(184 7)	(186 6)	(187 7)	(189 44)	(190 17)
(191 17)	(192 6)	(194 6)	(195 7)	(196 5)
(197 6)	(198 6)	(199 12)	(200 18)	(201 9)
(203 8)	(204 16)	(205 34)	(206 12)	(207 5)
(208 4)	(209 5)	(210 3)	(212 4)	(213 11)
(216 8)	(217 133)	(218 30)	(219 16)	(221 6)
(222 5)	(223 5)	(224 3)	(225 3)	(228 4)
(229 5)	(230 8)	(233 19)	(234 8)	(235 5)
(236 3)	(237 4)	(239 2)	(240 6)	(241 2)
(242 6)	(245 12)	(246 7)	(247 5)	(248 6)
(249 3)	(250 6)	(251 5)	(252 4)	(254 6)
(255 4)	(256 6)	(257 7)	(260 3)	(261 4)
(262 9)	(263 15)	(264 8)	(265 6)	(266 5)
(267 4)	(268 6)	(269 5)	(270 5)	(271 6)
(272 5)	(273 4)	(274 5)	(276 6)	(277 14)
(278 6)	(279 6)	(280 3)	(281 5)	(282 5)
(283 3)	(284 4)	(285 3)	(286 6)	(287 10)
(289 5)	(290 31)	(291 15)	(292 8)	(293 6)
(294 5)	(295 5)	(296 5)	(297 5)	(298 4)
(299 7)	(300 5)	(302 7)	(303 3)	(304 2)
(306 3)	(307 42)	(308 15)	(309 9)	(310 6)
(311 4)	(313 3)	(314 3)	(315 2)	(317 3)
(318 4)	(319 6)	(322 3)	(323 3)	(324 4)
(325 4)	(326 4)	(327 5)	(328 3)	(329 2)
(330 3)	(331 4)	(332 6)	(335 5)	(336 4)
(337 5)	(338 5)	(339 4)	(342 3)	(343 2)
(344 2)	(345 2)	(346 3)	(347 4)	(349 4)
(350 2)	(351 4)	(352 7)	(353 5)	(354 3)
(355 2)	(357 3)	(358 5)	(359 4)	(360 5)
(361 3)	(362 5)	(363 2)	(364 6)	(365 7)
(366 6)	(367 6)	(368 4)	(370 3)	(371 3)
(372 5)	(373 5)	(374 4)	(375 2)	(377 4)
(379 3)	(380 4)	(381 6)	(382 4)	(383 4)
(384 3)	(385 3)	(386 3)	(387 5)	(388 4)
(389 3)	(390 5)	(391 4)	(392 3)	(393 4)
(394 3)	(395 3)	(396 4)	(397 4)	(399 4)
(401 3)	(402 5)	(403 4)	(404 5)	(405 3)
(406 4)	(407 5)	(408 2)	(411 7)	(412 5)
(413 5)	(414 5)	(415 4)	(416 4)	(419 4)
(420 6)	(421 4)	(422 2)	(423 2)	(424 4)
(425 4)	(426 6)	(427 3)	(428 5)	(429 6)

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(436     6) (437     3) (439     3) (440     4) (442     2)
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(593     1)

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COMMENTS:Kopka J, MPIMP, Dept. Willmitzer |RI:1685 |RI:1685 |RI:1685
CASNO:168002-11-1
RI:1685
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Table 4

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258	319	352	364	211	264	299	377	289	245	312
294	308	341	250	340	312	210	287	318	277	276
287	300	288	312	294	227	309	315	318	272	284
280	296	285	179	291	197	291	291	355	298	294
227	257	258	270	321	256	295	302	219	303	260
237	237	205	276	260	256	220	267	363	325	254
205	317	264	233	330	324	194	328	306	337	170
231	371	246	256	252	253	264	287	276	318	276
252	257	260	295	279	265	289	245	276	254	278
247	187	236	241	311	292	215	248	167	255	252
228	232	243	241	192	202	261	253	232	180	288
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325	339	354	248	267	317	312	384	372	205	495
582	237	448	487	340	330	378	346	311	226	342
267	350	223	238	344	273	272	258	338	292	203
239	0	257	195	332	282	322	306	322	354	51
257	129	552	334	277	322	159	307	332	315	359
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189	326	329	257	221	300	284	284	191	119	324
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259	287	343	296	258	288	259	261	324	313	256
244	27	283	294	260	376	209	354	337	287	301
230	250	308	348	300	278	190	239	195	268	358
248	222	221	296	301	287	392	252	124	305	223
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248	323	376	268	329	331	294	273	303	297	272
299	291	279	246	325	237	322	353	328	281	278
296	313	328	232	332	230	324	323	336	301	299
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	219	198	200	201	212	159	199	193	8	209	193
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	147	171	263	145	184	210	714	139	340	19	229
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	14	212	204	63	0	211	69	11	123	81	84
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	298	384	388	409	235	311	389	246	328	338	330
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	237	254	313	357	362	304	392	320	110	295	288
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338	351	264	333	315	230	315	443	333	347	213
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296	324	404	290	279	297	196	196	278	303	296
306	311	325	273	289	186	322	341	333	310	306
312	307	273	174	289	233	305	308	386	321	319
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301	317	253	198	347	326	172	352	264	262	233
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342	348	329	296	309	307	325	291	339	334	280
332	102	310	316	294	394	323	359	422	331	335
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310	284	290	331	351	286	370	292	189	312	258
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371	384	275	319	328	158	301	578	323	323	252
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311	295	296	260	300	218	305	332	301	288	295
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229	263	219	273	272	250	277	232	289	288	296
254	111	318	233	297	292	242	234	32	234	261
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224	303	322	210	203	263	283	253	191	54	335
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193	207	256	272	259	280	345	264	118	292	240
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249	268	246	287	280	174	260	216	204	234	256
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617	232	234	208	570	594	218	203	326	635	222
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246	230	216	195	229	265	217	218	177	248	249
220	234	237	249	263	238	92	270	247	268	239
231	170	250	212	214	231	243	245	251	262	263
238	194	225	259	157	143	146	174	195	202	132
238	136	508	525	532	507	508	554	493	450	500
529	210	196	248	260	218	224	221	234	263	256
207	154	151	217	243	238	303	263	179	240	266
242	107	243	236	142	169	265	303	251	139	298
265	294	208	189	164	191	305	955	137	238	2
273	233	275	190	262	256	170	315	242	242	188
205	124	236	297	291	289	218	242	275	34	276
231	272	186	240	263	145	254	178	228	182	84
295	148	240	246	179	195	223	178	269	232	90
245	421	198	267	164	284	124	254	243	266	482
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47	301	262	202	246	597	125	274	199	98	323
221	320	209	206	163	193	241	227	270	215	208
243	243	192	259	170	285	240	169	259	271	228
281	240	179	229	462	228	142	210	200	231	287
431	401	158	265	262	266	151	232	292	231	193
107	220	242	226	258	570	369	525	209	536	278
463	494	246	251	274	517	313	253	56	206	511
224	521	436	251	237	74	264	139	243	271	237
422	358	323	311	258	306	265	291	281	218	

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363 375 269 276 442 247 461 164 486 303 515
145 582 619 327 486 392 217 449 203 41 597
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284 526 137 582 267 527 629 291 663 424 571
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309 93 330 565 602 676 396 471 619 313 278
226 300 574 516 555 522 258 357 435 421 675
404 402 468 600 563 460 528 524 219 402 393
422 397 118 518 500 142 512 84 510 545 533
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1315.1_1164EK04	191	235	207	327	325	176	790	226	286	999	
	264	212	262	353	275	255	806	231	300	313	288
	330	154	197	339	302	351	275	352	220	454	249
	237	224	181	251	221	217	262	381	307	262	286
	266	350	204	306	91	287	359	160	200	245	226
	339	219	253	227	240	300	234	274	247	217	162
	316	237	194	153	275	237	264	141	188	233	317
	234	243	303	241	185	264	129	233	250	246	247
	245	208	235	229	256	163	292	232	286	252	209
	236	273	249	173	238	217	237	236	302	231	232
	128	211	211	231	369	283	187	221	156	246	229
	213	208	119	292	254	209	184	247	155	277	215
	166	186	304	131	237	281	154	357	226	257	175
	183	293	233	219	218	238	204	232	221	267	249
	230	232	181	281	248	251	247	233	243	231	250
	244	143	174	249	278	236	214	149	98	154	161
	124	23	126	124	179	220	224	163	270	147	313
	277	315	134	296	191	790	313	321	970	190	249
	261	207	256	204	278	278	230	217	343	261	333
	374	210	234	300	394	250	341	421	276	138	261
	219	316	205	200	333	164	235	344	239	332	20
	238	0	271	180	312	288	356	269	215	290	50
	204	44	324	260	296	275	230	275	231	264	320
	209	249	177	209	314	251	324	191	308	308	291
	131	341	297	104	217	287	311	245	188	145	339
	221	296	312	181	283	6	226	136	259	106	229
	0	246	1	263	275	264	246	145	269	382	271
	220	270	233	224	225	198	266	171	294	220	229
	207	131	267	292	215	315	260	317	376	211	239
	183	170	326	228	190	273	133	191	263	153	494
	291	204	251	309	329	250	303	235	121	238	256
	259	225	57	220	251	2	245	76	292	244	236
	253	295	238	228	190	239	158	225	195	151	

1318.8_1185EK05	283	304	282	258	292	220	292	243	339	264	
	999	245	282	508	314	350	249	282	264	259	242
	283	267	294	306	328	309	316	240	328	304	339
	322	319	244	376	276	346	366	337	253	298	305
	279	368	366	224	212	254	259	208	193	290	299
	229	259	281	266	235	305	264	286	252	289	245
	282	273	304	241	313	233	265	267	237	281	301
	249	270	601	220	232	307	195	211	257	277	268
	263	268	275	219	272	207	285	295	293	250	277
	252	274	232	315	230	280	244	197	301	275	273
	215	256	254	261	202	276	186	297	270	296	312
	228	180	198	281	282	289	257	186	196	340	227
	251	272	277	181	227	329	294	284	199	149	270
	239	334	243	234	227	253	203	229	223	323	217
	230	238	252	286	269	234	273	215	260	256	288
	244	294	237	245	286	254	205	207	155	132	190
	16	154	186	240	303	217	323	146	221	274	290
	333	256	178	261	217	292	368	300	266	272	944
	309	348	276	331	328	309	199	371	300	295	321
	297	237	240	324	263	315	381	451	329	183	383
	213	336	266	326	306	134	238	282	341	218	153
	315	0	316	639	647	288	252	352	330	317	140
	306	266	298	289	324	341	191	300	311	285	294
	262	280	331	324	446	395	309	244	277	309	296
	221	363	317	231	284	322	577	301	287	372	347
	271	319	242	233	266	61	249	306	283	218	264
	0	244	264	279	273	325	273	178	301	243	310
	297	334	342	292	240	285	320	266	287	296	243
	276	73	252	315	236	342	235	331	356	297	315
	122	273	364	320	287	233	232	223	262	205	402
	253	243	252	301	321	257	355	263	129	319	257
	270	262	197	289	244	251	269	242	286	262	248
	231	229	320	334	297	326	294	297	276	277	

1318.9_1164EK04 377 390 131 368 365 470 320 204 429 212
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196 223 235 286 293 345 252 0 310 291 283
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1326.9_1185EK07	360	356	165	363	384	360	404	253	370	262
282	320	999	405	333	390	376	289	340	448	397
379	169	333	602	314	336	807	370	385	359	370
409	404	333	354	318	171	300	465	421	371	283
293	679	382	279	166	377	393	250	352	695	317
314	318	305	300	319	349	311	355	276	288	309
334	303	301	307	302	288	693	316	336	272	272
282	319	482	231	301	303	194	344	304	312	280
285	302	311	387	302	227	320	331	325	278	297
275	310	310	180	302	150	307	753	537	293	289
213	259	260	269	352	304	222	330	263	329	277
272	203	146	285	278	293	263	737	320	348	252
273	309	296	181	262	468	177	279	274	265	151
266	469	263	267	300	310	285	321	319	327	279
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272	164	180	249	318	309	190	270	106	242	304
292	232	259	283	150	217	266	260	254	161	360
368	316	115	727	338	404	387	262	252	357	108
929	363	398	250	294	424	249	332	370	230	305
378	503	364	438	272	355	394	405	309	188	346
260	316	195	295	426	174	278	507	306	308	144
274	0	269	241	302	377	294	340	330	357	19
134	170	379	361	307	284	303	330	385	302	355
222	304	384	284	226	564	313	383	291	305	339
535	292	338	242	240	305	407	271	207	75	351
201	316	354	200	554	358	309	228	292	119	306
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277	324	621	322	319	217	367	218	702	323	233
264	213	751	301	297	423	519	557	448	219	246
208	208	422	264	264	270	163	281	206	276	355
305	272	245	341	261	340	363	250	102	325	258
261	265	62	335	257	231	305	96	305	319	254
228	224	236	231	226	271	214	253	241	191	

1334.7_1344EC21	448	547	221	462	456	378	537	265	417	353
508	349	405	999	447	452	407	308	421	418	441
452	287	416	436	357	396	426	413	438	474	401
446	424	334	407	354	198	360	412	585	349	401
393	435	425	363	202	388	420	298	333	365	402
387	363	365	367	369	418	365	345	315	324	363
317	351	348	369	316	312	362	349	356	282	411
313	312	519	320	354	412	216	379	351	377	364
383	381	378	302	395	213	371	326	376	356	388
369	376	367	170	369	186	371	287	460	367	369
294	294	300	303	431	336	283	398	268	399	327
318	296	251	357	329	318	196	270	334	423	282
267	368	351	292	380	337	178	357	268	238	247
247	386	297	300	302	310	297	334	331	360	302
288	293	336	331	322	352	329	249	298	298	319
378	160	197	279	313	299	239	296	80	318	303
251	248	296	294	170	214	313	313	249	158	433
427	399	90	263	336	537	422	211	306	420	362
340	420	398	257	358	388	296	370	427	390	333
364	263	358	397	364	404	487	453	438	216	399
299	408	227	281	549	82	362	328	408	386	203
332	0	322	426	584	359	382	389	360	406	58
253	188	415	384	344	386	241	400	341	359	400
211	344	256	296	332	433	306	205	384	417	353
218	387	437	268	245	320	412	332	203	157	434
255	302	352	211	382	254	373	221	361	134	323
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283	386	370	352	242	273	330	247	349	321	316
276	54	350	355	293	434	270	420	423	274	310
157	237	440	322	296	341	224	267	325	295	436
231	278	361	393	419	311	378	311	135	325	316
307	298	132	289	290	97	269	155	313	277	273
271	242	292	275	268	314	252	258	216	232	

1336.4_2011EC31	349	339	212	310	295	281	313	290	492	275
314	346	333	447	999	674	285	627	659	320	304
335	290	374	270	303	469	335	262	461	322	511
492	493	575	594	483	221	438	329	329	302	339
330	319	505	268	214	418	344	239	238	240	505
289	334	329	330	282	259	329	286	350	278	312
248	454	354	316	249	311	231	343	504	322	354
327	379	331	493	439	459	174	395	465	431	370
376	434	401	349	380	250	416	389	409	417	425
401	423	382	194	398	194	416	181	293	416	410
229	367	366	359	260	326	157	536	251	537	446
340	208	183	419	362	401	170	226	312	313	382
260	257	289	222	301	172	197	317	278	224	237
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361	330	359	351	333	323	334	282	371	309	378
356	193	219	312	326	310	227	377	124	364	372
303	290	339	401	195	190	306	309	284	192	291
532	606	212	215	261	313	525	251	190	411	160
319	632	424	384	716	339	376	491	358	339	230
323	171	299	333	220	581	348	273	630	266	573
139	512	191	319	353	118	319	227	514	281	221
474	0	445	310	346	286	316	314	422	383	82
260	137	272	496	363	428	175	333	455	415	369
223	419	328	272	344	254	347	151	403	353	466
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333	403	384	209	204	308	383	214	345	202	314
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343	470	191	345	354	233	200	257	202	394	440
302	123	355	369	365	407	160	438	405	259	234
184	242	406	423	369	356	301	344	349	329	429
353	367	354	367	380	323	444	324	254	400	315
309	306	204	363	318	152	303	130	343	353	294
234	304	309	327	297	355	276	327	282	226	

1346.0_2011EC29	367	348	193	321	331	310	361	286	512	255
350	319	390	452	674	999	294	369	741	371	393
402	281	446	309	375	592	390	341	535	394	511
495	512	578	513	450	216	426	329	396	321	377
327	361	525	346	257	477	418	215	293	336	435
336	392	390	393	423	344	390	275	421	310	347
272	491	366	353	259	403	324	350	438	424	319
365	379	340	374	461	480	208	446	450	429	406
453	489	430	412	445	209	456	414	470	394	460
394	495	481	159	453	164	491	226	312	426	425
262	387	387	370	290	351	232	483	248	488	455
363	260	208	393	380	383	193	259	326	371	389
253	272	276	263	333	218	178	372	254	225	217
222	245	346	395	359	339	339	346	324	370	361
355	400	304	424	399	381	405	341	377	388	438
367	166	256	368	410	379	157	386	167	314	368
293	375	314	310	185	221	287	349	322	126	325
522	639	171	224	299	361	522	283	192	401	203
347	950	456	355	469	370	400	438	388	319	276
352	181	310	357	255	705	344	321	630	260	523
256	485	164	291	391	69	301	253	454	369	243
420	0	445	339	315	306	365	390	462	435	0
269	126	343	451	305	478	240	353	485	465	498
237	461	338	326	359	288	421	168	394	315	365
155	435	522	286	334	369	216	504	248	146	445
366	397	373	262	232	355	433	217	371	139	389
0	398	227	417	272	549	423	293	432	366	429
371	512	269	364	342	281	197	289	259	403	435
371	192	380	380	395	467	207	543	459	292	253
182	282	456	430	359	483	274	378	345	362	512
338	384	370	396	383	373	465	374	168	417	414
355	379	171	456	383	189	385	190	414	393	362
317	365	266	314	283	330	287	302	261	306	

1351.6_1344EC23	306	340	192	309	310	293	845	195	338	806
249	320	376	407	285	294	999	248	315	379	380
386	197	317	389	341	422	372	368	347	442	339
334	331	273	303	280	162	280	413	339	336	295
307	359	324	324	146	267	369	205	223	319	292
364	298	323	307	286	330	310	241	295	255	278
311	272	266	272	281	234	341	239	260	251	354
288	278	363	282	246	304	191	292	288	309	284
290	319	303	340	292	213	335	274	336	269	314
254	326	289	159	276	190	302	286	344	253	254
157	273	274	285	341	301	269	241	230	260	260
230	183	177	300	268	256	199	272	179	364	258
239	277	282	163	327	328	165	368	247	243	193
187	344	250	234	235	255	211	227	215	314	270
258	245	255	279	251	232	270	235	283	262	289
298	161	215	273	283	251	229	191	90	226	204
188	22	167	187	176	202	245	192	238	147	284
357	357	151	374	312	845	381	226	858	328	197
329	259	357	211	301	334	202	299	408	254	438
348	254	335	386	395	298	396	450	361	152	317
300	325	323	229	393	184	277	423	331	376	110
247	0	309	253	378	333	361	292	296	327	60
218	105	345	374	297	287	253	346	312	307	304
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197	346	257	254	266	291	330	357	207	172	367
233	324	309	224	348	198	324	225	307	221	239
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272	295	303	274	242	244	297	240	336	266	253
317	222	350	334	294	319	288	355	386	252	285
195	240	352	275	243	256	160	247	289	217	460
304	275	258	313	336	260	307	241	107	285	231
248	229	146	277	260	131	252	141	276	276	233
205	263	261	256	257	269	212	245	230	208	

1372.0_1288EC46	270	243	225	289	263	219	262	261	359	231	
	282	256	289	308	627	369	248	999	441	257	240
	267	283	265	216	253	328	249	237	308	284	330
	327	316	362	507	367	274	396	290	250	234	271
	272	292	386	241	186	359	364	216	219	221	318
	256	344	327	328	222	228	329	344	329	304	283
	323	336	335	287	286	342	192	320	347	252	380
	307	276	263	482	245	401	184	477	379	344	306
	330	323	312	203	310	237	339	360	340	442	332
	446	327	309	247	339	196	316	180	254	442	445
	226	284	286	317	260	357	170	363	228	363	396
	372	251	208	367	331	379	180	210	259	327	338
	241	211	301	241	339	197	239	333	253	190	288
	218	209	271	328	282	286	266	302	309	353	309
	350	362	409	367	359	422	353	320	355	330	362
	456	247	225	350	352	341	212	313	147	313	345
	266	215	327	264	230	242	288	297	330	243	267
	349	344	207	197	209	262	367	260	169	274	227
	295	340	289	293	887	268	263	439	307	287	237
	294	197	270	263	224	358	309	254	425	249	510
	161	421	198	239	246	105	275	209	290	276	136
	377	0	324	230	289	342	247	266	280	350	97
	249	180	240	288	349	383	226	374	418	360	357
	210	294	231	284	258	253	301	191	408	407	332
	149	344	369	296	280	308	205	302	195	212	398
	237	341	373	233	204	248	357	236	312	153	340
	0	316	159	277	231	443	310	211	305	286	405
	291	366	201	310	322	261	212	280	223	276	340
	288	59	244	373	302	295	164	299	297	276	250
	191	278	332	350	302	334	208	260	375	285	336
	265	317	432	334	335	281	350	380	332	362	304
	313	318	169	271	367	137	272	149	351	332	321
	283	297	314	350	298	320	214	312	262	246	

1373.5_1164CC54 366 315 262 349 352 255 310 257 421 300
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396 349 481 317 240 374 304 226 304 260 452
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227 389 307 298 196 346 318 285 630 348 311
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1379.5_1185EK02	402	403	225	370	352	367	389	258	419	313
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400	419	401	401	394	227	407	401	514	409	321
264	410	409	342	227	319	386	278	391	361	429
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318	352	321	342	308	312	346	326	336	282	360
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329	375	340	709	348	208	367	401	373	361	358
357	366	377	275	375	247	372	353	340	385	373
289	337	342	352	363	318	316	308	307	293	349
286	246	195	325	352	338	326	338	352	459	330
332	364	266	231	403	406	258	392	294	306	236
324	342	315	294	296	296	302	303	315	351	301
314	288	292	369	348	326	360	314	328	331	349
267	262	209	336	366	363	249	306	171	303	312
301	282	305	300	306	273	352	287	265	262	365
476	327	147	376	376	389	408	263	312	372	100
382	386	438	321	302	940	340	371	414	209	393
467	293	346	424	341	365	401	408	389	165	414
396	377	257	544	519	180	269	299	360	379	230
341	134	335	262	358	331	350	390	419	362	84
279	160	533	382	293	383	227	381	367	378	380
279	297	268	327	325	364	313	327	330	380	308
243	396	348	269	356	366	353	292	339	177	460
297	374	392	222	361	282	338	319	337	193	361
207	279	234	306	329	362	340	223	351	368	392
385	364	329	384	306	326	326	276	374	427	330
294	215	335	377	332	390	309	360	438	336	338
271	275	371	360	345	345	254	326	274	297	377
364	276	333	392	372	344	421	338	189	355	361
313	295	169	373	330	277	344	261	369	372	368
280	293	345	358	322	367	300	366	362	271	

1380.3_1164EK04	411	351	167	448	396	373	389	162	550	288
242	391	397	441	304	393	380	240	373	566	999
473	160	369	484	267	351	414	485	426	464	380
425	409	351	410	454	142	427	364	472	326	242
263	367	343	537	141	370	422	249	246	370	356
499	302	324	328	290	499	309	195	381	223	363
215	381	333	359	208	244	336	343	312	251	396
259	652	313	293	282	370	221	247	370	338	320
328	337	326	439	348	188	379	561	378	393	335
404	347	370	109	378	143	365	327	384	424	406
244	343	344	360	528	292	207	327	264	323	277
250	198	172	278	307	252	263	293	324	393	316
273	277	248	202	276	301	110	430	330	370	103
271	361	283	300	258	285	280	301	265	315	251
292	298	234	435	456	243	403	309	421	431	413
234	122	195	390	422	434	175	256	16	255	262
228	252	239	261	135	107	275	227	289	121	444
431	354	123	324	378	389	543	155	293	400	142
362	365	350	199	288	500	817	320	488	268	267
434	278	334	417	377	313	323	420	369	185	348
250	417	223	308	450	0	250	233	310	562	198
237	0	252	236	412	379	521	269	522	356	185
189	43	531	336	286	348	206	365	350	423	409
250	293	261	243	247	330	268	239	326	381	283
256	320	291	238	490	333	355	299	190	111	448
197	517	275	216	307	159	328	502	318	165	229
203	288	190	365	333	432	367	235	380	556	408
515	339	319	565	303	197	287	239	341	580	328
288	213	312	332	346	406	285	327	343	202	256
234	235	374	331	520	334	203	290	278	239	269
377	257	294	312	332	322	352	315	104	273	246
286	315	72	461	312	160	455	40	417	419	500
217	265	209	255	184	263	188	264	273	158	

1402.5_1164EK04	341	370	205	474	379	375	411	165	515	330
283	580	379	452	335	402	386	267	301	423	473
999	235	651	426	286	397	432	539	407	645	427
422	398	352	402	454	188	419	429	482	480	333
285	417	505	507	210	365	404	297	362	381	441
490	403	396	389	529	406	380	309	457	274	481
316	471	490	486	297	348	365	491	305	351	398
303	307	371	350	364	393	270	298	352	445	424
431	433	437	331	425	215	434	405	449	465	441
471	421	404	150	434	230	405	344	389	462	464
321	390	386	431	582	367	289	328	331	326	382
348	327	375	454	429	329	329	287	275	405	348
360	327	282	369	448	359	153	581	372	463	198
325	355	342	359	357	340	330	377	322	383	355
326	365	303	447	442	313	428	376	426	420	439
314	145	354	383	436	434	260	333	132	345	345
310	124	330	321	153	335	341	426	356	136	427
376	333	171	335	374	411	538	191	325	606	152
339	347	372	221	272	342	362	404	948	289	374
354	256	414	477	559	297	389	454	321	85	372
376	393	203	230	425	169	214	280	484	520	184
267	0	305	221	411	370	480	304	399	461	46
283	90	471	371	318	452	218	440	384	482	405
278	263	267	296	300	359	287	241	393	388	385
253	359	471	243	368	315	336	303	232	96	533
226	365	431	345	315	175	432	347	379	142	392
255	317	192	361	385	365	411	180	429	568	479
377	465	289	430	286	357	305	368	358	442	349
419	195	327	416	372	441	344	385	457	366	384
394	357	422	427	427	371	235	293	324	242	395
310	225	386	403	402	330	480	429	149	329	315
362	353	89	357	402	121	382	215	415	411	404
289	286	287	315	294	328	275	304	279	283	

1402.9_1344EC19	242	241	186	323	343	260	212	194	233	154
267	282	169	287	290	281	197	283	157	253	160
235	999	282	199	198	303	225	247	251	245	232
262	238	338	279	274	261	297	309	209	206	260
211	261	262	216	248	220	210	214	244	210	267
214	236	241	248	169	268	236	220	229	224	296
217	252	274	293	211	264	207	277	235	255	270
309	265	251	242	230	288	199	289	274	247	250
252	259	256	120	242	179	259	260	254	266	251
268	258	242	235	230	176	237	187	228	257	260
223	216	214	229	201	289	256	244	255	246	261
250	269	253	255	241	255	214	167	215	297	224
248	237	199	263	165	248	221	161	283	236	335
220	293	237	238	233	229	219	247	221	256	253
236	242	220	247	242	261	243	232	245	222	239
249	226	365	237	266	243	245	245	122	258	250
225	145	267	224	262	220	296	273	252	255	308
288	215	139	139	239	212	240	175	154	303	193
132	179	238	245	224	186	113	305	260	199	306
185	135	257	288	217	193	295	342	236	74	249
166	264	188	130	182	25	203	203	261	207	270
251	0	282	164	301	196	205	187	174	265	37
249	91	274	135	214	240	192	232	163	223	270
170	110	144	354	127	234	245	79	217	253	163
154	273	259	153	147	217	234	192	180	198	267
173	141	301	364	212	187	241	156	229	143	291
0	231	176	180	210	167	225	130	210	192	254
203	225	191	207	155	375	168	379	165	195	217
200	51	153	262	177	224	186	233	244	379	350
253	381	252	235	201	226	192	178	167	226	204
162	153	265	222	248	208	328	265	44	246	243
180	239	7	150	251	89	179	173	251	187	228
239	140	337	404	336	309	242	288	306	357	

1412.3_1344EC09	387	347	31	377	368	356	329	287	585	197	
	294	566	333	416	374	446	317	265	314	369	369
	651	282	999	361	264	460	386	385	503	418	514
	490	490	395	454	530	35	467	368	433	332	308
	372	368	505	351	228	402	340	306	413	316	446
	421	409	415	425	367	306	414	329	468	311	639
	327	517	621	653	302	383	316	646	309	381	340
	330	331	281	344	394	409	298	337	356	477	477
	488	491	473	292	490	184	476	450	490	491	479
	490	494	484	125	497	223	491	282	355	510	508
	411	429	433	464	393	354	278	460	362	459	428
	351	299	372	477	442	357	293	261	350	365	366
	382	391	297	403	370	195	146	392	300	309	219
	330	232	359	366	375	360	349	394	353	414	364
	358	427	307	453	447	392	445	420	474	424	500
	362	27	411	423	429	426	222	396	175	394	410
	368	285	379	406	46	371	311	490	373	26	380
	356	314	166	256	317	329	584	222	189	575	136
	254	390	385	224	299	346	336	539	653	271	331
	379	149	346	464	326	364	302	363	351	223	430
	306	523	150	203	388	3	339	301	466	366	218
	355	1	363	243	322	269	433	297	452	474	25
	260	128	326	458	337	493	178	363	491	506	449
	188	311	245	280	319	260	336	120	423	318	379
	156	438	541	231	446	269	202	380	236	0	526
	278	396	442	412	266	244	479	287	435	148	436
	275	304	143	377	275	342	482	186	484	406	476
	423	496	253	414	312	389	156	404	308	408	397
	338	52	314	397	401	488	250	385	471	398	389
	300	382	445	361	424	398	254	316	305	329	519
	300	326	388	423	421	347	486	445	171	294	355
	382	364	113	361	447	82	386	149	423	413	408
	263	302	266	302	292	357	305	330	278	327	

1412.9_1164EK04	462	322	168	439	424	577	399	205	355	339
306	346	602	436	270	309	389	216	249	476	484
426	199	361	999	293	322	503	436	357	456	300
359	329	269	326	290	147	289	603	420	348	268
263	566	311	378	174	348	408	276	367	587	297
360	309	313	299	353	586	306	319	261	287	337
348	303	324	335	299	253	582	319	252	226	355
243	238	483	237	282	299	208	339	251	310	298
296	309	311	362	332	210	279	279	290	286	301
287	274	257	164	261	172	261	571	499	287	294
234	238	239	243	396	275	254	283	227	280	223
227	252	225	269	260	241	202	559	353	384	219
234	307	314	228	338	465	163	356	297	299	124
233	537	234	273	246	266	244	271	266	320	253
213	236	230	259	240	251	267	209	287	274	292
282	121	292	216	268	237	261	249	130	259	261
157	114	266	254	117	174	265	274	231	110	397
391	337	175	604	559	399	372	130	297	390	221
531	268	280	173	243	391	212	357	411	195	408
447	404	393	415	371	269	440	545	275	179	317
317	295	182	312	412	59	252	510	282	472	142
215	0	216	279	386	326	334	344	255	353	42
200	135	562	280	362	280	231	322	314	289	331
199	256	333	305	255	574	238	344	250	339	265
443	301	315	150	192	271	453	258	138	141	367
184	208	285	282	516	148	297	182	286	101	292
0	221	137	256	464	254	223	212	254	357	312
220	271	612	280	260	272	325	295	590	255	209
255	28	584	270	265	414	490	464	470	272	257
250	288	484	243	234	269	183	210	226	235	348
232	218	246	316	298	296	362	231	158	266	224
203	261	71	266	240	189	239	138	267	240	217
239	217	229	227	188	243	104	238	249	202	

1419.2_1135EC00 253 256 250 317 303 237 302 197 287 302
328 222 314 357 303 375 341 253 309 305 267
286 198 264 293 999 318 325 239 271 299 266
285 292 262 252 250 282 331 259 290 275 366
327 301 299 260 220 325 308 194 267 295 261
261 265 264 273 287 248 257 279 218 290 259
265 226 259 264 281 309 288 253 277 273 278
268 281 315 257 219 333 173 233 454 271 262
265 262 248 265 259 197 273 245 276 251 241
267 272 249 302 260 193 266 244 309 263 269
272 263 269 281 234 292 207 303 226 293 226
261 242 184 223 201 236 144 234 211 277 203
226 241 236 227 246 275 299 266 267 220 256
209 289 279 311 299 300 272 287 253 301 279
309 251 248 282 270 244 277 227 257 282 273
284 288 208 249 270 254 190 424 103 416 426
313 252 402 390 295 190 304 264 253 278 297
311 318 164 192 248 302 306 171 237 275 193
266 275 237 482 318 335 268 292 299 218 265
277 219 294 305 260 347 340 291 264 174 261
266 271 206 140 282 78 315 305 277 244 230
269 106 281 287 299 302 276 296 202 289 24
199 110 269 223 235 274 229 277 264 251 306
179 207 432 316 199 282 245 254 198 294 242
180 323 306 185 240 280 246 292 245 257 258
314 228 233 200 247 234 276 173 243 135 186
0 262 126 208 288 235 284 269 233 240 301
231 253 276 242 284 243 208 222 269 267 210
225 20 253 266 224 275 186 293 317 278 254
145 229 320 281 255 266 218 229 242 176 280
192 291 232 273 283 249 335 228 122 268 244
218 268 112 271 256 56 180 237 264 239 209
245 267 344 343 299 301 352 328 281 246

1428.7_1344EC11	365	353	164	299	321	341	436	245	477	351
309	322	336	396	469	592	422	328	515	402	351
397	303	460	322	318	999	361	318	467	353	420
476	473	462	471	435	171	433	445	383	318	375
300	310	444	278	219	458	374	269	362	358	397
293	363	376	379	360	337	377	329	398	297	400
322	445	408	399	289	326	322	380	424	364	323
357	450	295	398	368	481	192	383	389	424	387
387	420	397	328	426	154	442	476	429	446	411
448	436	429	153	450	172	460	229	287	507	501
268	387	383	373	288	354	299	437	288	449	402
339	294	219	398	392	335	229	227	341	402	349
307	319	274	249	340	259	152	292	329	316	264
268	249	349	386	360	349	345	380	322	374	387
316	357	373	455	452	323	422	362	422	422	429
366	142	274	401	420	414	221	293	88	287	306
282	298	298	278	166	232	321	358	363	181	285
481	499	186	201	328	436	471	245	327	386	141
267	552	429	339	401	318	355	480	417	352	351
417	116	340	412	245	468	326	322	460	188	482
264	485	101	248	391	14	263	335	434	295	211
371	0	477	335	309	225	309	315	443	424	65
259	111	346	368	313	449	229	396	404	439	472
226	398	304	361	264	287	373	98	347	313	378
150	445	414	367	388	384	219	418	197	49	473
314	443	425	286	250	308	390	307	345	49	383
21	392	164	387	262	493	395	220	418	311	436
429	446	320	428	308	303	210	299	317	425	415
369	137	300	428	371	450	169	424	469	322	314
225	302	439	360	432	383	241	322	375	335	498
400	322	366	396	394	362	466	398	209	406	337
350	342	180	401	383	110	392	209	437	389	435
281	329	315	324	265	345	290	351	289	257	

1440.4_1185EK03	386	417	194	379	366	360	393	259	344	275
316	358	807	426	335	390	372	249	323	463	414
432	225	386	503	325	361	999	403	404	380	377
416	435	375	378	328	201	324	425	486	416	298
310	608	453	309	185	348	391	288	364	594	359
370	350	355	357	375	365	366	343	294	282	347
349	316	356	344	301	306	597	348	302	309	315
298	345	513	263	314	355	191	354	299	333	310
320	321	340	411	345	242	330	377	348	325	321
334	350	353	200	343	172	345	592	464	350	347
301	272	271	284	387	298	297	322	274	314	314
307	235	203	306	324	309	267	561	342	381	262
303	372	272	249	329	417	196	325	314	265	172
294	444	258	305	327	313	287	333	315	357	337
253	287	264	342	332	331	363	262	307	368	318
315	185	191	284	363	350	206	299	134	239	309
290	252	269	285	180	217	298	297	275	179	354
423	311	139	610	347	393	365	239	204	407	172
781	334	390	300	261	399	299	361	408	295	344
405	440	426	469	294	370	389	406	379	193	383
316	370	193	243	489	160	315	461	341	330	206
275	0	293	295	366	376	386	407	316	365	105
174	210	394	370	331	327	228	342	350	336	373
242	278	405	312	335	528	330	302	279	321	329
459	337	368	239	275	329	400	304	232	85	379
264	316	385	214	484	302	345	284	317	120	309
3	322	199	323	436	290	300	254	301	346	376
283	358	541	329	275	231	364	210	599	322	290
254	36	585	345	287	473	486	513	455	232	277
194	192	426	352	311	292	228	281	288	280	361
331	271	293	362	307	338	376	265	122	293	279
249	302	84	334	276	182	346	155	364	368	284
239	258	250	247	196	272	213	259	243	216	

1441.4_1344EC30	326	376	173	489	396	354	421	201	384	352	
	240	422	370	413	262	341	368	237	316	405	485
	539	247	385	436	239	318	403	999	347	638	307
	334	343	267	295	358	147	337	395	476	372	228
	258	388	376	569	234	326	356	268	298	401	306
	635	313	329	312	428	369	309	244	354	241	323
	238	344	333	323	246	282	388	319	251	302	319
	281	232	376	230	321	296	220	259	278	311	323
	334	318	324	346	349	282	306	315	326	358	291
	364	290	285	118	300	202	291	353	400	341	344
	235	308	307	331	709	300	232	235	302	232	262
	257	251	201	295	304	250	282	350	314	370	264
	318	308	305	250	368	329	120	575	285	370	233
	314	331	264	258	293	287	258	290	277	342	253
	253	290	220	297	298	301	301	239	310	322	319
	303	122	186	267	319	317	235	227	99	236	234
	320	223	222	228	128	242	306	262	273	132	470
	422	345	143	376	361	421	401	220	263	477	96
	382	289	311	230	248	336	419	302	569	204	304
	336	319	355	394	569	309	371	451	268	275	309
	283	322	257	216	409	118	226	288	333	624	220
	210	0	237	222	439	312	636	339	276	345	214
	232	91	449	289	292	377	190	378	272	360	324
	152	234	216	287	247	356	277	225	374	322	272
	265	300	356	234	244	292	349	251	254	96	405
	184	231	327	209	356	226	330	217	327	114	288
	1	232	240	270	380	278	319	254	341	690	377
	225	322	341	320	272	246	254	238	326	314	293
	339	26	308	334	304	354	285	361	365	271	267
	281	228	324	306	244	285	185	243	291	199	257
	246	214	315	340	276	309	340	289	139	273	252
	238	281	62	262	264	183	284	213	318	302	245
	198	267	253	250	225	278	274	265	244	245	

1453.0_1344EC12	417	376	211	339	359	374	403	258	736	220
328	453	385	438	461	535	347	308	408	399	426
407	251	503	357	271	467	404	347	999	353	967
962	955	425	511	596	257	541	387	427	350	312
305	340	635	312	240	368	345	264	367	325	444
359	490	495	502	309	299	491	309	502	317	561
308	589	593	567	300	344	307	595	432	368	287
361	455	339	352	472	394	209	355	410	497	507
518	538	510	316	539	167	640	503	638	497	525
501	646	660	167	649	138	662	275	314	502	495
347	514	512	491	308	413	309	635	269	634	410
414	265	249	518	480	360	314	290	367	377	342
320	360	306	294	316	318	158	275	280	278	168
343	284	366	414	379	356	370	391	366	396	354
360	404	399	525	516	353	521	374	540	499	569
371	167	303	441	495	493	230	334	104	352	356
301	274	320	347	171	189	326	321	366	176	345
447	479	176	251	339	403	725	228	187	482	169
325	472	543	276	358	360	361	458	415	237	351
351	227	404	502	280	472	349	349	416	248	506
325	621	166	225	389	114	273	260	577	285	253
325	0	321	291	367	273	382	356	622	536	26
271	120	336	468	336	508	223	299	563	571	462
353	345	311	326	393	298	373	242	342	313	465
217	506	549	266	360	312	241	406	247	68	496
361	466	556	317	287	333	523	311	496	91	489
7	537	138	555	287	449	550	251	587	305	516
444	533	276	478	317	305	290	336	285	491	350
350	183	353	504	552	596	342	448	554	319	335
176	324	533	462	459	454	266	343	308	364	584
348	315	337	471	454	411	484	367	176	388	365
307	359	83	519	370	124	463	152	481	501	413
260	354	296	337	259	358	281	373	321	274	

1456.9_1164EK04	388	370	236	544	458	390	474	291	487	454
304	397	359	474	322	394	442	284	286	405	464
645	245	418	456	299	353	380	638	353	999	367
355	339	305	349	437	224	415	444	493	531	282
286	386	430	521	242	358	468	273	334	380	358
561	441	441	444	557	360	435	313	447	290	331
327	435	340	336	303	340	361	360	289	358	419
267	319	395	257	306	321	240	307	271	402	420
432	410	452	350	454	250	376	427	382	429	393
430	362	359	203	390	227	364	323	459	429	429
308	357	361	410	658	317	310	275	317	269	334
316	358	280	385	389	292	321	327	356	335	317
360	334	310	310	554	349	199	685	368	431	214
336	341	303	347	313	289	322	352	334	349	279
303	340	292	371	376	351	364	331	399	358	393
364	185	230	332	378	381	268	285	82	291	298
290	204	280	295	169	226	348	350	319	159	504
357	269	172	329	387	474	524	279	344	431	145
323	294	348	225	270	347	436	315	639	207	357
309	280	354	416	925	317	434	474	282	262	321
497	385	239	289	432	301	273	331	397	540	244
261	0	296	238	451	437	598	339	343	491	194
363	98	460	341	345	469	239	453	364	448	401
252	250	291	289	281	382	334	258	389	391	414
271	375	452	247	331	271	350	293	221	151	553
207	336	406	242	375	269	430	277	412	190	380
4	275	236	355	437	330	386	294	413	662	471
345	392	350	439	285	285	290	249	358	418	308
352	185	304	391	346	434	382	360	478	310	338
352	242	498	368	369	368	183	288	358	326	378
294	253	386	440	406	308	429	396	156	326	260
329	301	90	313	352	188	379	201	387	400	361
253	293	286	293	243	320	256	301	267	298	

1461.7_1135EC00	386	347	64	322	351	348	404	272	687	249	
	339	470	370	401	511	511	339	330	463	412	380
	427	232	514	300	266	420	377	307	967	367	999
	931	923	433	489	538	59	471	360	439	319	318
	312	329	624	301	215	397	378	227	393	296	455
	344	455	457	465	347	297	458	314	484	311	531
	288	545	589	541	277	329	306	574	463	337	287
	360	429	308	362	438	366	193	365	401	492	482
	495	527	479	358	515	137	627	471	628	460	517
	468	632	663	62	650	118	664	243	284	478	472
	319	510	511	483	321	391	289	610	285	609	433
	400	262	255	528	473	353	220	248	364	319	347
	290	320	283	301	307	202	62	268	293	300	150
	280	224	356	403	366	341	369	385	361	385	350
	386	411	377	489	492	357	485	363	502	464	532
	346	49	251	414	449	460	227	354	125	353	377
	338	241	319	377	49	190	254	331	337	57	361
	397	461	92	221	318	404	678	260	205	494	23
	281	442	556	266	359	352	316	423	419	226	321
	337	96	356	485	288	523	317	325	463	240	515
	316	574	224	226	408	1	288	263	602	261	248
	423	0	350	289	336	270	344	330	586	492	0
	226	148	348	453	334	496	168	299	578	543	423
	300	389	275	281	389	266	339	68	368	291	488
	188	503	559	340	365	296	180	379	139	3	454
	343	456	567	263	275	327	505	259	474	20	477
	1	534	129	526	241	414	546	264	571	298	497
	417	526	249	480	296	235	142	243	277	492	349
	338	185	328	474	530	597	351	445	588	269	284
	197	234	508	452	437	444	276	340	329	353	628
	320	364	334	501	473	413	439	371	192	378	360
	311	350	62	484	359	43	415	109	438	472	398
	238	338	232	266	207	321	167	307	204	236	

1464.3_1344EC12	417	377	234	321	338	371	399	249	721	237
322	467	409	446	492	495	334	327	418	400	425
422	262	490	359	285	476	416	334	962	355	931
999	979	433	498	577	261	525	383	422	347	316
303	354	641	305	241	378	332	259	355	334	450
349	485	489	496	320	297	487	305	487	313	576
304	575	608	584	314	347	314	605	420	345	300
329	455	349	360	462	405	215	350	405	505	495
506	524	496	341	541	168	654	516	652	487	514
489	660	668	196	656	142	666	279	315	496	487
348	501	498	479	320	423	320	652	261	653	420
425	286	232	496	469	364	301	304	361	389	353
306	381	294	282	322	302	186	302	290	282	172
331	292	372	386	376	360	361	376	345	392	339
360	386	392	534	517	350	521	341	533	509	560
370	178	279	436	518	510	224	328	104	349	350
309	266	316	339	182	189	314	313	363	174	336
438	482	159	260	333	399	725	232	199	482	181
342	425	531	278	351	374	340	452	439	242	357
374	260	404	521	257	488	348	329	427	193	500
303	617	161	236	377	97	260	290	560	284	244
359	0	343	308	361	281	369	360	617	528	25
260	122	342	471	311	508	226	293	567	551	462
404	348	313	312	413	312	366	214	340	317	478
230	513	539	298	368	315	257	395	242	101	516
368	463	545	292	286	342	502	297	485	80	476
7	566	148	565	294	402	534	237	559	323	495
443	547	285	477	330	299	297	317	310	497	348
346	184	360	498	538	595	329	439	536	314	328
199	303	532	464	454	447	254	349	300	361	603
371	328	329	470	470	389	482	364	180	392	351
317	358	94	559	371	127	469	203	503	524	412
279	334	290	317	250	371	261	357	300	259	

1467.9_1135EC00	410	364	161	322	351	384	391	268	707	224
319	464	404	424	493	512	331	316	492	419	409
398	238	490	329	292	473	435	343	955	339	923
979	999	429	491	557	193	497	379	415	327	312
303	355	645	305	248	362	331	242	376	314	450
343	470	466	471	312	312	467	305	485	322	565
311	563	596	574	315	337	334	594	461	342	288
351	459	317	376	472	398	185	361	395	492	484
498	515	485	338	535	155	662	531	663	466	502
472	668	682	134	665	127	681	262	300	487	480
327	505	503	481	318	407	295	648	265	650	428
408	267	230	494	470	354	269	271	364	365	352
289	354	294	277	303	262	132	287	289	285	157
304	259	379	387	384	364	371	384	350	387	337
358	379	380	519	503	345	498	332	506	481	535
361	137	269	412	498	488	219	320	106	337	338
321	252	309	329	144	187	283	320	333	156	335
429	473	172	236	352	391	699	238	177	492	89
333	447	508	272	356	384	317	438	414	245	321
379	202	396	527	254	549	328	324	416	204	488
279	607	155	218	377	105	255	308	555	284	254
423	0	352	287	337	262	346	335	619	517	21
209	126	359	466	272	522	191	287	600	548	469
371	347	328	321	397	279	365	97	334	292	467
208	498	543	306	377	311	176	384	203	95	465
377	459	560	295	245	336	491	314	472	96	462
7	565	137	561	264	395	539	236	546	306	496
429	553	253	493	329	269	232	298	276	516	351
352	189	368	495	546	616	329	432	553	291	289
199	290	526	456	459	447	244	370	304	375	596
357	331	318	464	451	399	456	345	176	375	340
291	341	86	537	351	80	451	192	479	499	401
257	318	265	302	201	330	259	321	222	272	

1475.1_1288EC45	329	301	158	278	264	275	253	246	499	181
244	287	333	334	575	578	273	362	530	401	351
352	338	395	269	262	462	375	267	425	305	433
433	429	999	498	499	200	434	281	335	277	331
324	299	441	292	195	424	398	206	264	236	430
282	368	383	386	311	339	380	285	431	252	360
268	444	384	370	242	345	230	366	413	341	327
319	339	275	466	339	458	195	339	369	443	396
389	381	405	324	410	167	410	432	405	488	391
489	407	387	245	403	152	398	198	278	507	516
310	384	391	406	298	326	291	427	270	424	376
310	239	175	415	384	327	219	222	314	428	404
305	263	263	238	278	149	232	271	286	276	244
257	166	359	370	392	349	351	404	343	422	330
327	330	325	421	408	319	415	333	408	409	435
338	223	267	391	397	374	222	314	172	303	305
262	243	292	267	239	153	308	271	365	245	259
415	436	187	192	271	253	482	202	163	316	114
307	539	447	300	496	339	351	485	371	359	264
303	178	258	351	204	443	293	238	947	230	521
219	556	203	310	358	0	315	222	417	311	185
476	0	502	226	305	340	290	279	418	390	24
217	115	334	503	263	455	132	365	422	459	434
279	405	312	277	421	205	330	82	394	310	474
130	446	374	399	353	301	188	442	186	204	491
281	409	485	268	198	311	416	342	367	213	413
246	408	130	374	251	455	389	235	406	308	456
361	435	205	377	289	254	194	281	264	391	416
339	164	325	421	394	431	229	350	382	272	268
266	267	400	404	370	373	273	322	344	340	429
314	285	445	332	308	354	436	401	241	425	328
362	333	189	347	404	168	361	212	404	364	357
269	324	278	320	304	332	233	350	266	278	

1488.5_1288EC44	358	287	214	316	333	319	321	287	551	251
	376	301	354	407	594	513	303	507	484	401	410
	402	279	454	326	252	471	378	295	511	349	489
	498	491	498	999	568	236	487	356	463	298	395
	311	297	497	317	164	437	420	293	304	270	544
	340	510	528	531	361	320	531	305	483	306	381
	284	520	425	388	296	373	252	403	450	350	289
	391	424	311	433	437	470	232	364	466	466	478
	512	464	502	364	490	225	477	486	475	545	457
	546	475	441	156	450	185	446	210	273	550	549
	378	483	489	501	337	386	252	515	338	518	442
	430	237	237	495	449	459	240	238	402	385	487
	387	289	276	288	300	152	156	354	296	230	189
	271	180	329	391	341	331	338	362	345	467	349
	425	390	407	434	422	387	425	424	485	410	486
	418	157	239	427	403	400	170	405	321	474	418
	420	396	455	440	194	234	313	462	374	139	325
	517	529	123	225	299	321	556	284	228	355	172
	346	493	504	299	582	419	318	570	438	358	255
	390	179	309	365	226	545	273	248	536	291	967
	202	607	108	254	433	107	329	209	441	333	185
	494	0	402	314	291	286	335	253	460	552	46
	210	100	345	475	324	549	156	339	540	521	471
	216	404	381	239	343	227	350	151	463	355	491
	155	428	486	435	440	395	221	469	254	86	533
	328	491	441	266	201	345	551	345	505	210	334
	285	456	104	493	221	536	473	264	503	303	484
	440	535	207	433	355	222	163	276	254	446	525
	351	203	313	494	457	435	233	501	478	248	223
	262	267	456	472	387	418	271	320	403	320	476
	330	410	407	395	371	387	414	461	330	408	389
	423	363	165	380	475	200	350	147	414	399	407
	285	339	240	288	260	319	216	339	279	240	

1494.1_1135EC00	344	301	40	326	315	328	352	280	730	221
276	360	318	354	483	450	280	367	356	394	454
454	274	530	290	250	435	328	358	596	437	538
577	557	499	568	999	44	821	403	400	306	332
336	326	648	368	183	397	332	267	318	299	552
357	742	748	751	295	386	744	355	827	297	516
348	878	534	524	288	385	275	544	363	408	284
446	544	253	444	411	485	248	384	519	738	832
825	759	822	311	805	154	678	714	707	838	751
838	681	711	82	725	162	713	258	274	787	787
361	705	713	788	377	486	256	556	376	563	518
492	232	336	634	614	470	292	243	385	388	628
372	352	295	368	298	166	76	364	281	248	139
309	172	458	545	469	442	464	495	438	508	449
502	624	458	679	695	462	669	596	780	647	781
492	35	291	674	635	650	224	443	211	456	454
399	419	448	485	78	291	342	493	549	47	355
410	427	163	175	304	352	738	243	141	383	100
288	432	561	249	359	344	431	448	443	281	277
301	167	262	373	343	438	264	288	389	225	566
250	904	84	247	341	139	310	298	587	373	245
415	0	454	247	334	258	371	256	745	808	36
206	178	434	470	285	748	195	432	661	847	613
328	408	304	236	478	224	404	86	636	276	655
144	628	671	493	633	353	222	426	182	46	667
307	752	594	305	212	333	822	464	784	118	596
443	555	111	610	244	482	761	242	772	367	723
714	678	206	613	342	255	180	298	263	586	640
448	239	344	588	641	747	451	529	733	289	254
185	278	708	562	671	619	286	444	629	473	621
470	402	599	639	632	518	456	661	307	543	472
585	488	204	522	629	139	602	101	650	648	658
310	502	272	283	265	322	254	347	265	266	

1500.0_1135EC03	205	182	842	239	230	158	220	174	159	217
346	121	171	198	221	216	162	274	259	227	142
188	261	35	147	282	171	201	147	257	224	59
261	193	200	236	44	999	371	134	262	177	311
304	225	0	212	172	254	231	202	244	215	142
199	261	261	250	200	106	275	214	6	209	245
225	120	244	237	195	246	258	242	301	252	195
257	283	221	210	200	289	220	216	247	248	181
216	157	173	2	180	318	254	193	245	178	166
229	265	227	801	313	232	267	285	172	245	226
0	165	78	103	263	281	107	219	169	225	323
290	136	218	176	165	3	113	166	172	227	231
170	189	297	212	199	218	814	127	371	1	253
193	200	267	216	291	290	274	290	237	269	282
290	164	256	205	197	251	205	205	196	237	229
244	764	153	223	187	194	295	53	0	0	141
4	0	128	0	674	65	275	0	213	712	191
127	177	280	148	174	220	6	93	202	44	320
132	0	214	252	238	206	0	0	144	0	168
151	126	148	166	144	228	249	129	171	6	77
20	0	183	42	118	1	271	99	56	175	237
178	0	90	201	202	171	163	84	0	236	65
172	169	146	0	44	2	130	230	0	8	212
127	24	118	397	0	226	23	43	141	202	0
204	203	2	0	86	0	185	79	197	175	234
223	0	245	156	209	135	38	6	62	91	96
0	226	0	0	174	7	6	230	9	113	236
0	192	166	120	181	311	223	257	242	116	7
58	0	1	283	218	2	122	5	233	286	277
0	257	230	168	0	249	67	6	120	176	0
60	151	245	101	311	1	266	13	0	266	201
0	150	0	73	221	0	0	177	77	0	4
210	3	193	287	123	167	214	173	151	145	

1502.4_1288EC34 361 297 260 347 315 301 347 260 624 262
366 351 300 360 438 426 280 396 445 407 427
419 297 467 289 331 433 324 337 541 415 471
525 497 434 487 821 371 999 367 393 295 380
400 341 586 333 195 441 372 245 341 323 519
335 672 682 676 309 379 678 378 713 303 488
349 750 485 492 288 398 315 487 405 387 344
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727 655 719 292 712 201 617 643 640 740 632
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346 319 364 357 346 223 313 294 354 266 219
309 256 431 513 458 439 440 500 442 477 440
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387 394 409 418 333 300 357 474 504 318 332
390 409 241 180 283 347 651 197 171 340 212
254 379 574 277 345 335 409 392 416 258 287
293 127 272 384 320 439 359 325 315 219 481
252 799 87 241 312 44 344 253 556 325 256
425 0 427 298 399 299 333 327 639 715 195
240 235 428 383 270 689 207 444 576 749 580
325 353 264 359 456 272 354 119 608 323 616
127 611 635 411 591 266 271 366 198 123 630
364 666 541 278 270 267 743 444 700 140 532
429 496 141 561 285 401 677 240 679 335 673
646 671 262 565 281 318 199 308 266 538 603
430 117 288 605 587 663 389 516 641 332 297
203 305 655 528 613 597 283 400 586 428 560
439 356 620 606 644 472 472 601 265 559 471
523 483 190 468 552 137 528 154 574 571 595
367 461 298 340 280 333 238 335 248 284

1510.5_1164EK04	511	386	141	474	443	578	455	216	373	381	
	337	377	465	412	329	329	413	290	253	401	364
	429	309	368	603	259	445	425	395	387	444	360
	383	379	281	356	403	134	367	999	367	323	288
	309	415	333	345	221	386	372	271	419	445	327
	343	382	393	388	316	500	385	301	356	273	367
	297	365	385	367	278	303	425	371	284	265	402
	276	287	441	288	267	353	226	367	290	416	360
	387	421	373	303	407	210	356	386	354	384	421
	388	342	333	140	334	145	337	395	407	398	397
	235	282	284	308	373	309	334	320	246	315	294
	295	293	215	334	312	259	244	366	335	450	317
	264	338	329	233	341	451	130	308	294	309	234
	264	549	286	348	283	294	278	320	298	360	310
	273	315	334	367	367	314	352	290	341	368	358
	323	96	307	321	355	348	222	251	86	230	256
	172	61	219	240	89	212	288	265	306	102	455
	422	352	208	376	544	455	399	210	318	384	197
	387	282	314	208	279	324	240	375	431	276	480
	436	325	414	441	374	269	374	506	272	61	345
	292	409	248	283	343	153	284	512	339	362	210
	308	0	320	350	437	330	323	310	358	407	27
	296	110	550	319	355	383	263	380	330	396	427
	256	275	209	422	241	480	306	275	347	387	357
	291	401	372	256	261	275	389	263	225	140	477
	166	301	363	292	444	14	394	245	393	154	353
	2	305	109	297	398	279	311	126	334	342	441
	314	342	470	367	266	286	275	330	424	322	285
	305	36	380	322	311	454	429	365	511	310	314
	234	322	534	299	334	320	184	239	340	256	442
	256	220	376	420	419	351	404	367	203	343	289
	316	304	163	325	324	172	337	66	358	330	302
	257	273	309	300	265	330	196	328	326	233	

1519.2_1185EK09	353	304	270	375	333	323	379	204	445	307
253	385	421	585	329	396	339	250	338	514	472
482	209	433	420	290	383	486	476	427	493	439
422	415	335	463	400	262	393	367	999	407	240
213	368	421	429	204	326	320	308	280	302	368
437	334	348	360	377	464	345	259	358	218	390
231	352	408	387	240	256	337	391	295	283	307
288	378	349	237	312	342	187	259	276	333	265
275	306	310	466	300	187	377	403	362	357	303
358	351	316	199	326	176	335	317	343	387	362
232	320	334	361	498	325	340	290	289	290	301
267	262	176	306	327	244	251	331	261	413	271
289	381	300	214	371	352	194	464	351	353	152
276	342	273	250	275	284	259	269	259	319	267
246	255	245	373	364	232	352	285	339	341	345
263	206	229	339	349	353	179	241	36	239	252
154	58	190	248	196	204	283	221	279	200	385
396	369	68	388	331	379	481	225	286	407	199
376	389	382	261	306	473	388	442	479	314	348
373	281	372	454	429	337	395	425	401	117	464
291	374	289	347	986	124	176	239	337	457	147
284	0	280	269	430	301	485	324	409	373	150
245	57	506	437	375	367	206	392	381	390	376
269	307	280	261	371	360	335	238	369	303	339
226	399	301	266	316	341	324	341	231	171	491
278	379	341	245	298	235	314	327	311	122	290
12	323	214	345	325	351	359	138	350	538	367
348	354	348	391	307	299	333	281	395	372	275
313	179	356	363	327	383	332	356	403	264	316
299	276	372	290	337	261	221	254	280	214	385
318	270	328	313	316	311	400	332	152	350	227
287	249	120	338	315	210	343	211	378	364	328
214	255	229	273	244	311	238	276	251	229	

1523.1_1164EK04	347	393	187	391	347	323	345	234	317	262
298	345	371	349	302	321	336	234	309	409	326
480	206	332	348	275	318	416	372	350	531	319
347	327	277	298	306	177	295	323	407	999	270
276	362	381	306	244	343	397	261	305	374	314
395	266	268	263	516	326	252	282	297	232	304
270	286	313	303	277	252	376	308	277	248	352
265	298	393	254	322	324	260	276	249	293	255
259	275	266	353	299	255	324	303	315	285	271
290	305	290	235	290	220	303	329	412	302	302
279	255	258	276	366	305	303	245	332	236	266
275	347	288	273	293	290	302	338	248	346	246
319	351	290	307	607	346	230	553	363	392	179
319	348	276	272	305	327	280	313	319	329	286
282	260	298	303	301	285	306	246	296	312	298
277	195	208	230	293	303	249	231	98	231	237
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362	318	149	319	323	345	350	234	242	369	157
368	272	289	221	255	337	277	278	489	190	287
370	219	382	443	486	291	425	366	274	276	274
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293	301	366	331	232	282	290	238	358	333	221
312	154	352	284	267	329	295	313	344	272	277
325	228	349	272	280	263	262	274	225	253	276
278	256	263	333	307	307	346	274	159	248	241
235	260	122	294	242	216	298	198	299	326	284
248	224	307	271	259	295	283	288	281	243	

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316	312	331	395	332	311	380	288	240	270	999
408	331	335	197	195	327	432	204	196	268	332
210	318	321	318	226	367	310	266	346	254	272
282	304	316	272	280	292	272	282	341	384	351
309	267	322	302	271	368	179	222	293	306	264
278	291	300	290	291	227	342	344	342	384	287
380	324	311	305	299	269	316	197	418	386	389
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258	236	200	353	353	321	205	147	137	358	319
255	254	241	218	218	269	279	261	190	150	248
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368	264	244	312	308	293	203	278	160	153	266
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329	304	137	262	237	316	403	306	272	279	275
263	382	313	283	340	366	192	349	349	293	354
258	271	269	316	234	281	341	304	363	211	418
136	367	157	343	318	37	405	401	320	224	149
322	0	373	305	348	395	240	326	348	333	202
277	51	403	409	181	373	282	290	342	348	356
286	352	273	289	397	295	391	247	282	346	289
143	384	380	184	271	348	295	353	225	193	454
214	323	285	242	310	120	283	280	308	211	287
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296	332	303	328	323	277	302	292	262	337	310
316	114	238	399	334	339	232	361	327	271	298
221	266	274	284	319	282	258	277	306	248	364
268	306	356	301	336	276	380	324	315	335	392
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386	288	257	327	274	315	228	303	270	271	

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	303	303	324	311	336	304	400	309	213	276	408
	999	306	385	246	214	460	474	194	224	265	285
	252	231	241	222	241	276	219	243	297	197	248
	246	313	262	253	246	210	253	256	295	265	621
	250	221	287	256	251	305	197	266	298	313	263
	292	323	288	240	306	193	333	276	342	240	319
	253	316	301	254	245	203	270	204	549	250	252
	265	278	280	281	255	225	227	268	227	263	315
	195	255	179	279	288	257	156	177	193	260	240
	236	206	252	231	243	271	224	248	230	169	232
	211	348	235	221	266	261	243	285	286	329	254
	238	233	266	258	238	249	254	217	269	257	286
	272	211	217	208	262	231	202	171	160	152	181
	198	220	185	167	230	182	249	232	213	214	301
	316	250	147	242	264	269	389	261	273	277	244
	308	300	291	272	326	305	199	315	312	191	288
	264	280	259	308	244	302	343	238	342	237	314
	135	359	228	358	285	74	974	354	353	182	195
	292	0	354	240	297	458	244	272	324	279	123
	287	93	301	271	204	290	350	308	336	323	286
	202	372	229	264	311	279	292	195	278	605	270
	151	361	271	263	236	296	266	302	245	258	365
	206	331	311	214	402	187	328	277	268	125	250
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	280	324	286	305	254	253	328	248	213	284	220
	252	73	262	327	257	305	240	352	312	255	295
	191	243	277	282	247	246	178	271	205	276	346
	305	229	264	422	440	268	326	251	212	303	273
	274	249	109	274	226	227	257	109	269	294	234
	254	223	273	290	263	277	207	254	197	256	

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368	383	679	435	319	361	359	292	349	410	367
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354	355	299	297	326	225	341	415	368	362	331
306	999	335	280	166	351	445	256	382	660	358
336	329	311	320	347	319	316	357	292	308	334
340	319	328	338	327	295	667	305	229	262	328
252	276	608	284	278	357	184	357	319	352	320
315	329	326	350	333	213	322	307	315	315	339
321	316	274	187	302	192	301	658	548	345	344
253	295	292	297	343	310	218	360	267	364	331
293	313	180	312	293	294	211	677	293	407	303
289	318	321	251	326	473	184	292	273	249	201
251	490	281	306	305	304	269	306	318	352	294
276	300	311	324	311	289	316	266	306	311	314
308	173	177	289	321	308	201	258	102	254	277
260	250	264	251	173	263	320	280	281	172	379
375	310	50	701	297	375	357	203	242	390	236
635	334	276	244	326	363	252	364	401	259	323
323	485	345	372	314	310	445	470	349	220	309
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229	137	331	269	365	342	269	361	363	331	340
219	312	386	300	288	616	334	425	338	349	342
525	319	331	299	286	283	527	332	214	149	376
209	318	320	176	606	252	345	243	312	82	367
0	292	140	255	547	261	279	196	323	354	357
291	374	664	307	292	239	466	220	672	298	348
282	37	662	337	308	448	491	574	450	237	271
159	203	458	306	325	321	268	263	299	269	346
259	297	319	347	347	329	349	293	238	311	277
311	322	145	298	287	167	328	114	331	286	319
290	276	256	274	237	301	193	273	254	230	

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641	645	441	497	648	0	586	333	421	381	335
385	335	999	458	213	418	376	259	410	335	682
376	538	535	541	365	288	529	289	590	282	440
257	617	468	453	245	361	360	453	417	351	347
304	421	350	400	451	431	215	386	422	510	537
546	490	551	367	544	129	549	546	525	674	504
676	533	545	164	539	150	554	301	377	637	642
337	571	558	568	402	429	281	513	338	518	613
492	249	234	726	672	534	260	298	368	342	436
309	380	264	318	353	181	137	337	283	314	156
321	234	318	374	352	313	324	399	397	421	397
325	433	418	507	509	392	497	410	564	501	569
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343	428	714	247	461	353	315	443	478	549	294
347	14	353	425	323	530	357	314	448	300	511
325	658	171	281	363	8	391	306	889	473	199
445	0	399	287	325	284	386	381	593	538	0
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346	424	385	279	386	255	326	74	489	340	759
159	467	552	464	447	284	205	403	101	125	526
292	548	505	285	274	331	550	334	545	38	575
15	512	23	513	304	433	606	269	604	403	572
471	712	272	558	325	249	141	266	309	556	489
355	205	422	545	542	618	302	508	541	314	224
227	249	503	494	509	442	321	335	464	371	582
381	303	439	450	440	387	416	452	334	524	387
423	380	213	391	456	77	455	234	476	474	455
249	409	245	259	270	249	233	287	193	260	

1560.6_1164EK04	275	261	258	409	332	299	331	166	403	306
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507	216	351	378	260	278	309	569	312	521	301
305	305	292	317	368	212	333	345	429	306	197
246	280	458	999	128	286	287	289	243	271	276
560	300	312	296	336	393	294	234	347	223	269
237	340	240	269	205	248	246	258	279	251	291
277	328	251	250	267	293	248	215	276	287	298
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235	305	306	331	680	229	183	275	263	272	274
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269	298	268	264	289	256	183	479	264	305	161
289	304	248	276	247	233	251	282	282	301	244
248	277	223	338	341	275	324	269	358	347	340
277	181	173	313	318	338	180	255	71	255	258
248	139	258	242	173	182	263	289	252	191	367
347	332	55	183	346	331	402	168	257	341	115
325	309	340	188	271	322	414	302	509	219	227
321	159	288	286	443	281	306	350	332	169	324
192	329	233	190	388	70	188	222	366	900	146
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295	252	235	214	221	252	247	228	366	286	266
142	266	298	261	285	305	251	284	208	78	415
139	334	271	187	246	314	300	245	337	106	366
8	271	69	282	256	323	309	351	321	670	373
309	309	238	508	257	199	219	220	275	504	237
312	225	152	300	310	340	176	278	355	239	245
256	220	315	294	284	280	236	261	281	232	272
294	238	277	295	265	297	303	285	136	295	237
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163	214	211	238	215	272	178	235	192	210	

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212 306 166 202 214 257 146 186 240 227 141
210 248 228 174 220 219 185 234 240 242 215
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320 223 190 205 261 195 192 168 184 192 189
173 199 227 197 171 179 176 206 230 190 228
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187 199 210 135 206 110 237 217 195 219 215
213 179 178 180 249 174 306 220 226 221 187
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317 153 182 168 161 218 194 56 208 231 240
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378	362	424	437	397	254	441	386	326	343	327
460	351	418	286	207	999	428	327	306	322	387
303	297	316	309	320	281	295	346	319	369	281
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301	390	342	364	354	234	347	417	346	358	386
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314	290	353	348	341	302	346	322	330	360	360
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304	232	250	186	299	221	392	280	317	236	304
380	456	211	280	313	299	428	298	282	288	141
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316	307	343	372	250	368	348	320	488	219	442
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346	241	330	381	312	381	231	380	411	367	339
333	261	404	353	356	350	315	318	283	330	413
347	321	346	476	461	298	445	357	306	445	379
330	309	231	314	365	189	386	242	361	366	339
322	345	455	492	396	457	335	453	420	294	

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332	331	398	420	332	231	372	372	320	397	432
474	445	376	287	230	428	999	213	264	339	343
350	283	284	284	392	313	277	280	301	237	247
289	277	275	255	256	273	323	275	274	325	419
257	315	356	325	296	332	204	326	268	335	251
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276	269	270	289	334	250	303	248	262	243	316
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343	265	342	354	347	351	337	238	345	350	328
350	187	232	317	349	333	184	253	129	262	267
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366	282	126	323	327	370	440	242	328	325	162
352	443	356	254	434	338	410	360	436	223	342
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259	242	206	293	267	202	245	271	308	261	204
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257	193	190	174	197	306	215	251	282	285	299
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262	322	239	197	243	252	272	218	123	286	147
232	101	282	154	223	186	204	317	307	200	284
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159	197	253	214	264	268	212	184	213	286	241
213	228	265	240	185	300	215	270	302	241	231
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189	267	265	307	240	204	212	199	215	229	179
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296	308	346	290	319	139	276	297	283	255	298
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283	235	159	319	321	255	394	240	195	449	146
301	241	330	263	276	409	231	379	392	218	409
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208	282	308	314	249	355	349	290	279	302	258
233	286	322	257	228	272	303	253	301	217	380
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327	158	338	387	285	341	274	346	379	344	350
207	292	325	271	243	235	286	258	231	227	349
270	221	327	297	328	257	438	279	218	315	298
255	266	190	271	296	177	283	260	305	328	269
257	304	349	373	345	343	269	331	327	322	

1636.7_1135ec00	333	313	210	338	328	345	348	174	327	245
290	278	695	365	240	336	319	221	260	361	370
381	210	316	587	295	358	594	401	325	380	296
334	314	236	270	299	215	323	445	302	374	268
265	660	335	271	194	322	339	271	333	999	261
342	263	270	268	372	285	262	328	284	251	264
332	297	263	273	291	262	788	271	225	257	348
231	292	566	264	246	308	189	354	255	292	230
234	255	253	329	262	238	318	346	311	298	250
298	291	268	195	292	170	283	712	633	313	300
237	254	254	258	323	275	240	276	245	276	252
232	266	157	271	276	262	247	766	274	392	280
289	306	262	190	302	580	180	286	325	313	217
273	545	242	258	282	280	272	294	321	318	282
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284	162	218	272	287	283	234	196	135	234	234
237	176	229	245	180	193	245	254	226	174	308
359	317	87	774	334	348	344	164	193	321	103
732	326	257	243	270	315	253	341	399	227	351
334	594	328	377	312	314	444	413	234	139	285
270	326	214	223	346	213	261	522	306	310	199
215	0	249	236	344	355	303	445	302	294	155
255	102	339	242	345	305	311	362	307	316	328
223	275	332	308	227	642	288	492	287	352	275
613	282	289	244	296	271	500	283	232	160	342
200	304	292	231	715	152	283	232	258	29	343
1	227	141	284	635	248	284	222	297	308	323
311	324	729	328	220	242	410	259	721	320	310
313	31	810	309	264	412	591	551	463	240	288
251	246	416	208	330	247	183	214	274	242	319
231	263	283	314	316	287	382	266	199	292	236
288	267	115	251	248	195	324	84	310	328	303
233	210	253	269	236	303	232	269	258	222	

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	299	424	317	402	505	435	292	318	452	429	356
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	450	450	430	544	552	142	519	327	368	314	332
	285	358	682	276	200	387	343	254	345	261	999
	310	469	453	460	328	335	456	300	491	245	417
	252	517	426	425	244	348	270	414	362	313	277
	342	391	302	360	476	423	197	347	389	463	477
	480	447	492	336	477	218	455	446	461	614	450
	616	453	436	183	462	179	444	252	308	617	620
	366	457	453	478	303	492	227	409	401	411	588
	576	247	309	685	634	654	277	256	334	404	471
	369	325	260	387	330	165	175	343	293	246	195
	332	191	331	346	362	337	317	384	362	418	397
	349	443	315	497	493	399	464	485	489	457	490
	417	153	215	469	450	450	189	447	228	435	456
	401	357	412	442	200	323	305	501	429	167	337
	575	414	93	269	284	317	482	256	198	463	138
	294	407	731	257	416	346	356	428	452	581	279
	323	127	300	370	268	425	273	292	422	229	551
	218	558	123	342	322	120	312	281	637	291	200
	463	0	384	265	306	262	332	352	479	515	21
	184	103	345	438	255	480	159	339	447	510	431
	280	367	232	296	337	246	321	129	396	264	721
	149	397	532	313	467	316	209	394	180	89	511
	272	506	405	222	221	344	493	261	448	219	414
	342	384	120	404	242	460	483	214	482	333	496
	452	680	227	429	323	225	178	236	267	423	533
	357	76	354	412	402	450	229	432	442	240	227
	208	230	439	408	425	376	274	330	421	344	458
	341	317	417	381	369	343	404	469	294	469	364
	467	354	195	436	511	196	389	165	456	432	469
	247	374	255	262	279	327	265	339	268	231	

1641.7_1164EK04	315	376	219	452	344	345	385	213	422	339
229	367	314	387	289	336	364	256	293	355	499
490	214	421	360	261	293	370	635	359	561	344
349	343	282	340	357	199	335	343	437	395	210
252	336	376	560	320	303	350	348	278	342	310
999	343	331	337	371	325	320	248	346	265	317
277	360	330	319	240	299	312	320	258	298	314
253	325	326	231	371	286	364	262	295	320	316
343	328	329	269	328	231	324	351	345	337	325
334	330	327	194	348	351	348	289	342	328	326
303	301	303	326	770	274	235	262	318	260	268
239	217	258	314	293	238	347	288	350	307	285
342	311	248	297	329	265	186	525	246	328	170
356	287	263	281	277	240	263	276	261	304	236
273	288	248	348	347	335	342	314	333	342	326
290	162	218	304	357	357	214	259	74	269	270
277	166	260	245	159	221	358	285	264	157	447
353	341	176	280	348	385	428	224	277	407	111
346	239	324	234	281	280	466	290	538	189	274
324	226	339	394	537	302	291	381	310	173	292
224	322	248	165	407	157	248	248	304	552	313
229	3	248	158	368	332	969	285	339	385	46
237	75	370	271	278	339	191	337	327	355	340
198	255	217	256	270	309	305	131	359	281	278
234	329	326	228	353	311	310	252	251	99	432
133	370	347	240	309	208	333	274	332	238	293
141	300	251	290	340	326	310	299	328	722	367
362	315	286	381	338	275	252	248	312	392	276
326	137	264	301	286	356	274	341	347	283	312
253	247	345	315	346	299	226	219	285	232	260
242	231	307	292	278	281	373	321	224	286	236
282	271	76	344	313	125	380	227	339	350	341
196	237	290	268	285	315	322	309	303	265	

1652.8_1288EC27	278	271	198	313	289	312	305	209	551	219	
	259	293	318	363	334	392	298	344	341	339	302
	403	236	409	309	265	363	350	313	490	441	455
	485	470	368	510	742	261	672	382	334	266	318
	231	329	538	300	223	297	283	225	350	263	469
	343	999	967	978	297	289	975	296	792	265	480
	293	776	504	481	262	334	262	515	303	334	281
	349	374	258	343	335	346	216	351	435	643	887
	882	692	885	223	841	154	609	522	650	684	668
	709	604	630	224	651	188	640	249	257	641	643
	303	617	631	746	337	470	210	420	319	422	499
	449	188	309	580	588	443	290	267	306	397	582
	351	361	199	335	285	266	203	354	230	248	187
	322	247	380	452	420	395	388	447	398	430	392
	413	539	410	573	584	413	564	489	692	588	702
	432	227	297	561	571	593	212	392	274	481	406
	451	416	433	478	228	318	359	493	471	256	318
	395	329	134	254	305	305	594	229	201	312	144
	311	343	500	252	359	333	291	390	407	257	288
	311	256	302	395	372	328	293	299	265	140	524
	173	702	136	205	290	115	209	216	484	310	256
	345	1	392	232	291	233	362	302	545	931	29
	300	164	343	350	289	660	243	404	561	800	509
	288	299	227	250	395	229	348	179	574	288	651
	225	550	584	417	480	251	247	285	264	214	585
	175	577	609	299	215	265	921	388	864	176	573
	356	528	154	566	250	370	661	171	704	348	661
	535	586	247	527	288	300	277	318	233	504	598
	453	201	318	529	561	597	403	468	632	324	341
	209	305	626	443	515	498	289	370	609	382	569
	327	317	564	536	512	474	428	572	307	502	410
	506	419	171	458	533	150	526	244	580	586	504
	249	407	304	389	296	364	285	381	322	324	

1660.4_1288EC27	307	277	200	332	310	321	327	218	535	253
281	299	305	365	329	390	323	327	326	355	324
396	241	415	313	264	376	355	329	495	441	457
489	466	383	528	748	261	682	393	348	268	321
241	311	535	312	190	316	284	206	353	270	453
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309	779	515	483	265	345	264	515	307	361	293
361	396	292	375	355	394	179	353	458	642	898
894	693	911	249	872	161	616	521	654	699	672
713	622	636	203	668	154	643	237	262	652	654
302	650	667	757	353	490	223	429	301	427	480
539	224	303	572	567	431	273	226	332	406	575
335	353	224	355	314	272	179	350	247	250	189
304	260	418	499	458	444	438	494	423	449	418
461	524	392	572	581	404	543	480	706	566	693
387	197	285	545	559	575	202	404	288	477	414
465	417	440	481	201	309	337	511	462	207	334
392	359	134	232	308	327	570	220	206	323	152
300	349	502	252	322	339	317	417	396	236	277
317	255	330	404	377	330	288	310	276	202	536
205	687	147	197	295	69	214	226	461	320	240
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296	169	337	345	326	664	229	387	552	793	525
281	303	249	253	416	243	363	167	578	282	647
198	564	579	424	472	269	248	352	235	161	584
256	571	582	284	219	368	933	385	889	173	540
350	550	172	583	252	387	664	194	703	357	645
527	590	250	510	239	283	276	301	232	493	593
470	243	285	545	590	621	383	463	637	300	307
210	282	640	450	514	555	319	406	599	422	580
362	356	557	549	527	503	404	560	280	492	400
489	462	201	437	528	180	495	196	558	557	472
266	413	275	358	272	337	222	354	299	341	

1666.9_1288EC25	290	266	201	311	287	313	315	198	545	227	
266	291	300	367	330	393	307	328	330	358	328	
389	248	425	299	273	379	357	312	502	444	465	
496	471	386	531	751	250	676	388	360	263	318	
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337	978	984	999	312	290	982	301	816	253	480	
301	782	513	474	255	335	258	511	306	348	295	
359	395	284	380	347	395	181	342	463	637	902	
897	691	909	239	869	144	619	518	653	700	669	
718	617	633	206	664	133	642	243	256	688	690	
292	654	670	756	353	484	220	432	304	431	484	
522	210	316	576	573	435	271	252	315	406	579	
327	351	209	346	296	278	183	343	237	265	182	
304	257	402	491	444	430	425	484	410	446	408	
458	543	394	587	597	393	561	491	710	581	706	
384	205	298	561	571	588	225	393	292	467	406	
452	400	427	470	208	313	338	508	473	215	311	
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354	0	401	234	315	240	344	314	549	947	29	
290	166	348	348	290	682	238	400	561	796	541	
277	298	230	237	423	236	361	179	572	288	659	
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401	547	173	585	245	390	667	168	709	358	645	
531	596	243	515	236	282	265	316	228	498	592	
469	246	298	547	594	620	406	469	642	292	325	
229	304	637	445	514	540	307	392	593	408	580	
364	355	551	553	530	501	403	578	293	492	406	
498	454	195	439	536	182	504	208	572	573	486	
252	416	268	364	266	330	214	343	284	346		

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235	340	319	369	282	423	286	222	310	384	290	
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320	312	311	361	295	200	309	316	377	516	226	
241	347	365	336	261	320	392	266	257	372	328	
371	297	344	312	999	324	307	262	326	218	301	
239	303	312	302	270	262	327	295	260	253	318	
224	290	375	212	314	294	205	259	251	300	244	
254	289	296	329	280	268	298	297	292	286	279	
279	279	248	189	246	201	264	247	393	298	300	
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230	328	231	283	294	239	271	253	207	338	228	
309	341	268	252	555	340	198	475	364	343	194	
298	332	255	257	261	275	241	280	256	318	247	
230	238	305	269	264	229	276	232	264	277	270	
196	191	226	210	291	278	216	224	82	220	229	
213	108	206	192	174	197	327	267	245	157	327	
368	297	133	377	323	278	352	221	275	355	111	
337	392	334	258	309	359	205	372	536	234	329	
310	309	385	368	488	305	467	341	317	134	334	
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252	277	320	310	304	263	303	257	310	288	245	
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317	255	298	337	264	246	237	273	233	264	282	
288	275	279	282	271	271	378	268	171	300	202	
263	236	102	240	261	94	259	256	290	307	257	
280	245	289	286	271	326	298	310	291	215		

1681.2_1164EK04	549	328	159	379	314	626	346	229	356	300
305	387	349	418	259	344	330	228	294	514	499
406	268	306	586	248	337	365	369	299	360	297
297	312	339	320	386	106	379	500	464	326	367
276	319	288	393	195	281	313	251	288	285	335
325	289	274	290	324	999	275	266	285	214	337
272	307	346	352	243	307	308	343	309	280	356
247	322	370	273	258	362	182	318	301	291	319
321	278	336	563	327	212	303	387	289	348	268
351	286	285	139	305	203	293	274	345	379	371
202	277	286	306	350	305	303	277	211	274	277
271	290	125	288	284	266	190	229	290	432	276
241	347	302	215	328	391	137	322	392	372	152
213	396	252	302	258	256	257	306	284	305	282
238	260	312	347	338	304	312	269	313	296	312
292	142	288	311	323	326	220	250	86	264	259
215	246	275	231	155	168	316	239	265	147	340
394	388	31	304	616	346	371	156	223	385	183
290	328	310	173	280	451	385	397	360	278	379
487	219	422	418	264	251	465	459	318	197	333
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318	0	348	287	450	283	353	313	320	318	109
212	89	960	364	311	330	203	302	323	319	403
214	236	210	312	414	328	284	217	290	329	322
170	433	400	137	301	256	307	328	218	185	482
248	317	287	286	294	188	312	283	306	60	325
9	216	85	258	307	299	313	185	327	333	354
311	310	319	320	366	296	292	305	328	341	286
241	27	256	308	278	347	241	355	352	274	283
346	306	383	301	331	293	199	230	250	232	369
265	221	353	331	320	285	346	324	187	267	303
298	256	101	285	313	149	319	135	364	314	323
317	259	302	312	256	300	189	309	285	188	

1681.9_1288EC26	284	263	199	313	291	303	316	200	529	234
264	283	311	365	329	390	310	329	326	348	309
380	236	414	306	257	377	366	309	491	435	458
487	467	380	531	744	275	678	385	345	252	310
219	316	529	294	192	295	277	204	348	262	456
320	975	981	982	307	275	999	303	788	252	473
303	773	505	467	257	329	257	504	308	347	291
359	389	283	385	352	390	183	337	452	633	888
883	687	900	226	858	149	608	517	643	692	664
709	606	624	214	651	166	633	241	255	648	649
282	615	632	752	350	479	211	421	298	424	480
521	212	296	567	563	429	272	246	317	403	574
329	355	209	329	303	277	186	344	230	258	183
300	262	402	492	443	427	424	481	407	445	406
457	519	378	565	574	389	535	471	701	564	687
373	205	287	542	552	572	214	389	284	461	402
447	398	424	467	210	311	341	506	458	217	317
393	365	114	242	291	316	567	213	211	304	154
322	354	513	245	327	331	287	404	391	232	284
316	267	307	392	372	328	280	293	271	165	545
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353	0	399	244	321	235	337	307	555	932	27
302	165	339	342	321	660	227	383	553	788	522
274	322	220	244	419	239	363	175	576	278	646
218	565	566	418	468	269	253	343	250	151	578
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388	529	181	562	247	381	658	167	697	353	638
524	584	248	509	239	284	276	305	227	495	585
466	244	294	528	558	604	401	462	641	294	326
226	295	629	444	502	539	312	388	584	406	574
356	354	553	549	525	501	404	557	276	491	398
475	445	190	435	520	168	501	210	551	553	469
266	407	275	362	275	335	222	345	285	347	

1708.9_1344EC71 223 252 193 217 279 231 267 651 371 274
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248 296 309 301 262 266 303 999 327 765 202
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316 292 297 328 215 306 213 327 289 322 300
287 249 198 337 333 289 364 336 330 364 317
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	487	485	431	483	827	6	713	356	358	297	346
	297	292	590	347	184	319	301	210	301	284	491
	346	792	793	816	326	285	788	327	999	268	471
	333	930	474	472	266	420	264	475	325	399	283
	380	422	245	407	346	450	197	412	469	648	834
	819	684	803	286	822	112	724	631	743	803	663
	802	724	748	32	761	152	751	231	255	768	770
	342	750	767	874	363	473	260	502	345	509	554
	466	260	303	688	652	434	282	220	326	372	620
	338	331	274	340	294	151	32	373	289	288	198
	302	167	462	522	474	451	469	512	453	461	465
	486	646	428	653	669	443	640	565	763	649	743
	457	10	299	654	611	619	209	436	309	478	448
	422	410	479	509	9	308	309	510	546	12	358
	331	384	139	203	257	354	667	217	176	321	100
	283	418	488	159	333	332	390	395	441	275	251
	254	133	239	357	352	333	264	275	306	189	506
	243	738	248	238	280	58	297	254	560	327	226
	382	0	415	240	332	260	362	309	609	780	44
	206	164	348	376	270	800	181	448	618	942	578
	307	411	319	208	407	199	351	109	685	269	685
	162	550	706	514	565	262	228	402	167	192	648
	247	668	654	284	199	239	850	437	846	113	666
	415	625	118	664	278	425	823	219	840	396	743
	625	685	172	647	350	247	149	307	248	620	636
	485	243	335	661	701	725	453	532	682	280	263
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	435	363	608	618	605	520	429	665	333	498	460
	568	489	202	420	615	176	591	155	619	629	601
	318	445	258	319	280	293	221	330	257	294	

1719.5_1344EC71		249	245	209	226	249	222	285	578	329	217
	289	239	288	324	278	310	255	304	219	299	223
	274	224	311	287	290	297	282	241	317	290	311
	313	322	252	306	297	209	303	273	218	232	254
	197	308	282	223	192	369	237	223	281	251	245
	265	265	266	253	218	214	252	765	268	999	266
	803	270	293	262	853	622	269	240	371	674	241
	650	290	280	297	244	384	197	293	285	301	264
	277	265	253	170	277	175	299	307	288	307	259
	299	276	272	206	270	225	286	269	255	281	279
	257	259	260	273	256	322	259	304	252	314	218
	281	195	234	250	244	244	300	280	314	338	251
	240	283	221	226	215	267	165	222	222	184	204
	292	250	515	588	525	521	503	562	521	535	511
	482	231	172	268	280	233	252	236	257	280	253
	211	131	161	251	269	253	284	252	106	269	259
	279	81	260	240	210	223	323	303	263	142	239
	277	355	242	230	223	285	311	580	194	256	272
	295	238	238	277	291	279	171	337	294	237	292
	294	236	274	352	274	283	303	335	307	110	309
	196	271	222	207	231	143	173	262	255	240	142
	270	177	220	306	303	193	253	417	253	270	46
	246	287	233	253	228	255	243	239	265	272	553
	210	235	337	230	309	256	662	220	244	248	221
	190	384	223	171	234	731	285	302	244	149	340
	228	282	288	248	257	281	255	264	248	204	290
	220	213	183	274	258	333	236	180	263	270	292
	276	236	289	281	561	250	220	258	277	286	240
	526	463	225	260	243	236	187	230	305	249	238
	87	282	275	292	269	602	411	530	269	532	322
	410	455	271	286	307	528	358	278	134	245	527
	233	541	486	262	271	156	268	207	262	244	239
	487	387	387	417	342	382	327	367	348	244	

1722.2_1288EC39	363	273	193	243	260	323	275	210	533	162
245	503	309	363	312	347	278	283	294	336	363
481	296	639	337	259	400	347	323	561	331	531
576	565	360	381	516	245	488	367	390	304	272
248	334	440	269	189	281	247	230	322	264	417
317	480	486	480	301	337	473	202	471	266	999
239	475	946	969	258	280	281	931	295	297	283
275	342	288	320	363	318	166	279	359	428	424
427	425	432	291	418	171	483	455	468	439	432
434	469	462	228	466	167	458	207	243	468	456
313	418	420	443	285	437	255	438	306	430	402
404	263	313	447	439	335	256	206	256	397	369
338	327	192	355	353	267	198	352	240	258	177
277	282	331	314	333	340	310	349	323	420	301
284	349	290	505	508	252	483	378	463	462	471
235	216	451	405	488	473	228	282	203	244	294
257	332	231	300	216	270	303	339	381	230	256
361	297	171	249	295	275	537	219	197	493	149
276	341	391	240	346	331	293	603	504	329	353
416	244	506	582	256	306	301	349	355	89	410
247	555	230	227	409	21	217	203	416	320	141
334	0	355	231	347	240	328	288	506	528	27
248	130	367	429	248	462	239	319	614	481	421
280	327	253	254	344	248	343	204	372	289	416
211	427	418	304	394	291	257	393	223	245	522
237	464	461	447	213	256	448	382	426	147	418
399	430	169	434	227	339	458	154	464	293	482
425	441	238	397	286	356	227	450	257	391	384
399	190	279	384	397	408	291	393	408	356	390
222	434	414	358	425	338	286	317	360	305	550
312	263	349	384	360	319	421	421	181	374	310
405	366	207	433	404	90	449	167	513	501	382
232	361	299	340	330	358	231	359	308	307	

1723.3_1344EC71	258	242	223	209	303	234	318	617	372	316
282	239	334	317	248	272	311	323	227	318	215
316	217	327	348	265	322	349	238	308	327	288
304	311	268	284	348	225	349	297	231	270	282
246	340	257	237	173	341	289	302	269	332	252
277	293	309	301	239	272	303	924	333	803	239
999	337	268	237	787	617	286	250	336	678	308
604	268	271	348	254	387	234	269	263	318	302
319	298	309	217	329	175	309	357	301	330	282
328	290	264	259	264	225	284	311	292	306	307
303	301	305	336	228	315	227	300	270	298	268
299	225	182	318	321	279	323	325	316	332	302
297	274	227	217	233	304	191	258	218	234	201
330	274	496	546	518	515	497	554	525	530	507
484	256	298	297	306	271	293	259	317	305	310
289	174	182	261	299	294	262	258	186	286	260
310	211	245	274	266	257	357	291	284	204	263
273	312	222	274	242	318	350	624	267	255	193
308	218	242	287	328	292	179	313	304	223	326
254	249	248	310	273	291	332	334	300	141	305
277	334	251	237	263	175	230	315	246	219	133
282	156	301	277	293	260	265	370	286	322	114
305	303	284	263	301	355	288	302	296	333	554
265	266	317	257	317	277	678	300	279	297	256
243	364	290	216	254	654	267	327	339	152	375
270	325	306	256	277	294	325	290	333	204	302
177	275	183	288	298	320	282	198	313	246	332
312	333	326	302	569	268	282	255	296	307	296
506	442	282	316	286	310	245	326	384	291	286
170	299	350	268	305	575	396	499	275	531	332
400	471	289	304	314	564	396	323	221	308	484
266	528	487	281	307	190	289	212	300	303	282
445	404	444	487	396	454	335	418	421	311	

1726.6_1135EC25	319	291	99	338	328	299	325	232	700	237
273	353	303	351	454	491	272	336	389	352	381
471	252	517	303	226	445	316	344	589	435	545
575	563	444	520	878	120	750	365	352	286	304
313	319	617	340	199	366	277	218	263	297	517
360	776	779	782	303	307	773	337	930	270	475
337	999	513	486	266	406	288	504	386	407	281
372	485	245	415	375	458	216	419	482	680	797
791	723	812	309	789	142	756	664	778	800	684
801	752	785	107	813	179	796	231	267	786	788
347	787	801	881	370	476	236	516	338	522	556
435	262	281	706	677	418	302	205	351	376	587
351	341	279	332	296	154	122	385	269	247	210
315	186	436	495	455	427	458	481	443	464	432
458	604	407	657	676	418	650	541	740	655	725
426	120	325	670	626	633	189	437	289	443	448
402	393	450	497	135	307	312	509	535	146	377
391	394	111	194	274	325	718	215	162	374	137
277	490	526	230	371	357	399	407	475	265	293
277	145	254	382	324	402	313	300	399	143	522
242	821	249	253	308	59	317	268	584	334	210
393	0	430	284	312	216	386	311	677	772	47
220	153	352	440	268	796	196	435	621	980	592
326	391	295	242	412	235	377	113	612	275	626
165	539	700	503	555	311	195	422	185	206	643
280	695	667	328	200	287	820	397	792	152	697
410	648	127	677	247	432	845	223	860	389	727
651	697	187	664	370	280	169	362	209	639	590
437	246	387	691	721	754	466	552	687	291	261
199	342	666	566	657	591	309	422	607	492	621
459	357	589	623	617	514	496	642	306	538	436
544	451	206	469	602	185	600	176	636	635	598
310	447	266	348	292	337	235	355	266	317	

1730.5_1288EC39	352	280	204	303	311	346	279	234	565	194	
	304	490	301	348	354	366	266	335	307	321	333
	490	274	621	324	259	408	356	333	593	340	589
	608	596	384	425	534	244	485	385	408	313	316
	262	328	468	240	227	350	275	263	355	263	426
	330	504	515	513	312	346	505	250	474	293	946
	268	513	999	936	288	265	290	948	320	286	269
	276	346	290	352	380	346	215	334	378	447	434
	441	452	443	211	429	193	539	473	526	480	459
	476	527	514	242	510	219	511	246	247	472	458
	339	473	477	476	319	475	230	491	309	484	409
	417	293	346	468	463	345	291	237	287	395	386
	350	375	255	390	358	282	240	349	269	297	195
	330	282	327	337	352	343	339	393	338	415	314
	303	370	347	508	510	309	481	381	468	480	476
	298	240	435	408	513	510	258	316	200	296	321
	310	325	286	307	265	293	353	371	380	298	308
	376	237	197	211	320	279	581	219	143	502	137
	255	346	396	244	387	306	267	590	506	256	335
	432	189	517	574	285	340	306	363	367	200	452
	298	590	220	200	422	109	257	201	443	304	203
	351	0	372	258	325	232	344	315	539	540	29
	281	109	362	436	276	453	242	313	583	520	421
	309	294	205	278	386	240	358	150	388	279	415
	217	465	477	266	414	247	240	403	240	191	533
	250	506	526	446	215	177	451	376	425	195	461
	406	484	155	493	223	347	493	178	519	310	512
	463	492	229	459	284	384	237	440	301	452	395
	374	52	306	448	460	454	321	390	440	396	400
	230	431	417	443	461	360	278	310	402	346	545
	313	308	370	409	393	358	458	429	255	381	341
	392	363	162	468	396	104	486	236	507	514	394
	253	361	356	383	370	387	315	391	363	302	

1731.6_1288EC30	364	271	185	242	269	328	272	208	545	153
241	518	307	369	316	353	272	287	298	342	359
486	293	653	335	264	399	344	323	567	336	541
584	574	370	388	524	237	492	367	387	303	272
253	338	453	269	197	285	255	225	320	273	425
319	481	483	474	302	352	467	206	472	262	969
237	486	936	999	251	281	288	948	298	300	288
274	346	271	311	367	324	174	286	366	437	430
435	434	439	293	428	178	483	462	469	445	442
440	469	456	247	467	167	453	211	243	474	461
321	424	428	459	291	427	251	447	315	441	400
406	240	318	457	442	341	258	212	252	406	379
342	333	195	367	352	260	215	347	254	274	179
277	280	328	322	331	337	310	349	321	420	308
288	356	299	510	514	263	493	388	477	485	486
241	235	459	435	517	497	230	294	211	249	306
264	350	237	314	235	266	304	352	391	253	258
368	300	174	248	303	272	548	218	192	507	143
276	349	394	242	347	336	288	610	508	338	356
393	247	489	567	257	311	304	347	373	93	421
246	573	229	229	401	21	216	204	423	317	150
352	0	362	231	349	239	329	305	518	531	27
249	127	376	435	253	471	243	326	624	488	429
279	287	252	253	360	251	349	214	378	289	422
203	440	420	306	413	295	245	394	207	248	539
240	480	469	453	214	251	454	382	432	157	428
393	429	165	432	228	342	464	161	467	298	481
440	449	235	404	280	361	228	456	261	401	410
403	188	284	388	405	418	298	390	415	363	399
228	438	422	355	436	340	282	309	366	299	556
321	267	355	389	365	318	431	436	191	378	315
413	369	209	432	429	86	455	166	526	512	393
237	368	311	345	335	362	233	362	309	305	

1731.7_1344EC71	211	230	206	254	265	207	306	570	309	275	
	313	261	302	316	249	259	281	286	196	308	208
	297	211	302	299	281	289	301	246	300	303	277
	314	315	242	296	288	195	288	278	240	277	280
	246	327	245	205	171	368	256	228	274	291	244
	240	262	265	255	270	243	257	746	266	853	258
	787	266	288	251	999	601	295	231	351	677	262
	601	288	314	305	242	405	188	263	275	330	257
	260	254	240	153	250	172	298	280	284	271	243
	253	276	263	212	267	230	275	288	309	252	251
	243	260	264	277	241	322	223	277	251	291	231
	278	200	241	264	259	260	256	311	302	332	235
	247	273	256	243	240	288	182	281	241	225	166
	257	299	530	581	549	545	510	576	546	534	509
	498	227	201	265	275	219	263	232	259	314	257
	225	150	167	230	280	263	281	276	110	277	271
	276	23	266	239	215	162	320	308	272	160	280
	285	298	258	275	204	306	309	575	245	246	256
	314	187	241	244	282	250	188	310	326	246	257
	296	259	291	350	293	257	321	366	279	14	291
	245	252	264	235	275	191	209	289	259	215	111
	272	195	237	330	307	246	256	403	240	289	61
	268	305	258	211	257	230	217	275	255	281	523
	231	247	338	249	303	296	677	228	221	276	195
	207	373	247	139	231	656	314	333	240	166	318
	227	307	310	232	307	235	260	230	251	183	279
	225	268	191	264	304	322	254	175	283	249	294
	279	235	327	275	542	230	239	258	320	264	246
	547	460	240	259	230	260	209	263	320	231	198
	171	275	312	282	249	587	424	561	248	534	302
	423	486	259	321	314	536	356	279	98	248	554
	224	558	497	239	255	162	238	204	268	259	255
	485	400	372	387	332	388	320	361	366	235	

1735.8_1344EC63 264 283 185 282 261 260 262 594 404 237
233 242 288 312 311 403 234 342 346 312 244
348 264 383 253 309 326 306 282 344 340 329
347 337 345 373 385 246 398 303 256 252 292
210 295 361 248 179 338 273 312 285 262 348
299 334 345 335 262 307 329 634 420 622 280
617 406 265 281 601 999 251 309 370 709 270
634 369 235 380 325 429 265 303 330 326 357
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305 290 297 350 335 265 199 370 331 365 320
273 195 218 324 308 307 332 257 284 401 371
311 324 256 254 267 264 238 277 219 220 239
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353 241 271 332 365 361 289 297 203 324 301
361 255 324 292 303 287 381 337 382 266 300
313 368 216 209 257 262 414 602 168 253 149
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248 212 249 308 275 396 371 322 356 216 357
184 391 336 254 294 105 213 233 320 256 156
381 109 363 212 323 270 311 336 333 347 186
308 369 306 265 338 460 255 378 306 420 742
330 289 270 317 308 272 717 255 358 314 288
144 422 357 225 345 630 241 327 351 227 438
268 373 353 316 222 268 356 300 365 272 383
192 304 209 320 252 484 307 224 328 352 447
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559 454 234 344 305 369 158 318 399 353 335
190 350 325 372 349 665 392 548 307 592 322
490 535 432 323 365 545 498 442 307 370 569
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265	292	693	362	231	324	341	192	318	346	336
365	207	316	582	288	322	597	388	307	361	306
314	334	230	252	275	258	315	425	337	376	272
253	667	360	246	176	273	323	254	346	788	270
312	262	264	258	327	308	257	304	264	269	281
286	288	290	288	295	251	999	283	208	262	292
250	235	519	280	247	285	194	322	222	255	234
243	259	264	338	264	197	286	307	299	279	268
282	297	301	208	281	181	286	689	556	273	271
238	236	236	249	320	244	182	264	259	265	273
226	226	189	292	303	285	244	775	264	375	237
286	304	229	210	319	552	197	278	263	295	172
256	489	236	232	247	250	249	266	290	308	244
206	252	234	248	240	233	261	228	253	263	270
251	189	245	215	267	248	200	224	114	214	235
237	171	209	253	197	205	292	229	232	203	315
325	269	68	785	309	359	324	194	215	325	173
728	303	281	257	251	301	206	313	357	258	315
299	557	317	375	298	288	420	386	261	193	267
287	319	196	174	364	222	260	491	334	275	155
226	0	294	250	354	332	317	395	255	289	29
242	93	335	262	310	290	262	303	317	294	326
220	280	374	327	266	635	329	414	245	311	260
640	309	301	163	258	275	471	265	283	172	325
211	260	333	250	651	201	248	206	240	141	272
0	233	168	303	532	255	244	152	257	331	294
236	337	733	286	244	259	390	238	744	286	248
286	23	784	303	246	435	576	543	465	264	280
220	222	390	266	280	245	152	232	241	261	323
241	255	252	329	324	286	345	246	94	280	274
243	238	111	238	234	185	250	110	297	292	240
248	236	271	279	272	300	234	289	273	241	

1745.0_1288EC30 377 281 194 261 295 328 256 203 576 141
267 484 316 349 343 350 239 320 285 326 343
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256 305 453 258 206 326 275 233 317 271 414
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269 350 266 323 365 337 197 286 361 449 457
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1759.0_1344EC20	289	293	278	247	253	273	290	326	447	188
237	259	336	356	504	438	260	347	630	336	312
305	235	309	252	277	424	302	251	432	289	463
420	461	413	450	363	301	405	284	295	277	341
295	229	417	279	230	459	274	210	236	225	362
258	303	307	306	260	309	308	369	325	371	295
336	386	320	298	351	370	208	310	999	362	346
387	347	233	514	345	513	176	322	354	372	336
329	367	341	308	383	205	380	333	376	332	358
333	380	369	319	377	266	374	143	263	376	375
258	359	359	359	284	272	207	449	260	448	382
268	186	177	370	333	311	206	181	288	312	246
276	257	240	223	247	247	344	251	182	191	274
259	208	319	323	327	320	307	347	333	412	318
316	321	345	331	328	293	332	299	327	313	321
295	369	263	318	332	322	217	251	217	259	256
238	289	251	278	358	170	404	287	299	378	266
398	464	169	165	254	290	463	316	166	319	141
332	455	361	278	465	350	304	419	304	285	261
297	190	272	356	218	568	322	278	479	214	440
183	401	250	286	353	114	285	251	348	302	167
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270	164	349	451	317	402	264	317	407	368	395
279	380	262	357	360	213	369	176	309	356	404
115	392	419	250	267	368	164	502	248	222	410
305	341	356	337	187	238	360	239	360	188	337
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319	377	255	300	401	350	248	346	244	326	290
298	193	280	416	389	443	146	378	404	335	315
153	335	375	366	307	391	274	294	265	340	376
299	338	370	370	357	336	453	329	263	399	396
312	303	134	371	333	150	308	279	335	361	247
371	328	383	428	389	412	355	426	353	336	

1770.0_1344EC63	245	276	229	304	296	214	255	635	455	233	
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	351	255	381	226	273	364	309	302	368	358	337
	345	342	341	350	408	252	387	265	283	248	384
	265	262	351	251	190	358	325	211	287	257	313
	298	334	361	348	253	280	347	707	399	674	297
	678	407	286	300	677	709	262	299	362	999	271
	721	328	224	344	282	457	204	370	325	332	336
	340	374	333	207	322	152	364	385	352	363	349
	363	335	333	254	354	276	345	193	205	379	379
	290	329	333	379	304	308	180	344	302	347	301
	288	234	262	339	333	304	264	288	333	320	344
	276	254	240	258	248	149	208	277	267	283	200
	273	152	604	670	628	608	627	654	607	608	654
	582	339	308	333	351	334	314	319	352	358	355
	318	189	243	328	343	340	286	296	197	298	285
	376	315	297	299	238	292	316	406	311	240	312
	319	349	234	196	219	255	453	640	154	294	103
	258	424	317	330	255	304	233	339	363	203	248
	269	136	219	309	305	364	265	264	391	152	330
	201	377	201	257	284	136	283	221	343	274	175
	321	241	332	271	231	200	305	309	368	378	43
	237	320	262	283	197	395	165	290	293	399	573
	203	352	373	300	236	189	977	112	383	231	267
	140	374	434	243	292	778	174	366	216	179	404
	241	371	361	294	165	276	366	248	333	201	349
	177	292	208	345	218	388	351	170	365	339	378
	360	376	186	310	524	297	143	281	228	344	379
	548	521	189	324	329	371	141	371	368	303	268
	215	322	310	352	361	631	455	608	449	641	334
	574	554	335	360	368	656	452	376	181	335	628
	318	617	508	302	353	94	312	149	328	306	323
	478	494	347	384	313	367	347	355	315	319	

1782.6_1185EK08	312	310	208	436	368	272	344	222	317	317	
	301	340	272	411	354	319	354	380	311	360	396
	398	270	340	355	278	323	315	319	287	419	287
	300	288	327	289	284	195	344	402	307	352	351
	621	328	347	291	228	430	419	245	298	348	277
	314	281	293	295	318	356	291	281	283	241	283
	308	281	269	288	262	270	292	275	346	271	999
	219	250	343	330	241	301	180	358	282	284	258
	267	278	269	371	302	205	285	298	301	306	265
	308	299	271	247	284	225	272	223	525	325	329
	268	263	261	271	322	242	314	271	261	271	276
	228	310	159	265	257	218	217	240	240	336	245
	281	309	298	245	426	334	246	365	325	298	251
	245	409	247	280	273	257	235	287	255	316	267
	262	262	295	305	289	295	312	271	294	287	310
	291	231	277	278	325	293	223	238	185	200	244
	257	249	217	208	272	198	338	287	265	253	408
	371	394	194	238	314	344	349	216	290	307	202
	271	309	322	244	443	356	302	313	381	216	391
	336	330	295	374	356	281	438	370	303	487	284
	352	333	256	402	324	152	624	395	305	293	175
	272	0	283	261	372	427	336	348	330	302	173
	349	137	376	272	353	350	532	369	313	304	302
	219	315	265	356	309	337	307	256	286	974	202
	209	357	292	203	246	268	279	284	283	320	471
	186	260	378	262	397	191	281	181	261	154	340
	4	274	170	252	519	312	256	220	271	318	368
	250	277	322	282	220	325	274	296	275	304	267
	314	144	301	346	303	311	213	317	354	339	306
	313	287	327	323	296	316	224	289	264	257	314
	296	218	302	395	420	295	416	339	185	300	320
	285	284	152	264	306	209	268	135	306	298	271
	255	237	355	408	373	365	265	352	310	260	

1813.4_1344EC13	294	248	237	286	296	227	317	571	380	234
249	283	282	313	327	365	288	307	398	320	259
303	309	330	243	268	357	298	281	361	267	360
329	351	319	391	446	257	391	276	288	265	309
250	252	304	277	194	340	257	225	285	231	342
253	349	361	359	224	247	359	613	380	650	275
604	372	276	274	601	634	250	269	387	721	219
999	308	237	364	257	414	201	331	331	328	384
388	323	373	201	374	182	317	384	306	404	334
405	303	292	243	308	280	291	209	238	369	367
259	339	344	377	255	270	218	321	259	325	294
288	217	198	327	303	287	266	270	299	338	346
265	247	267	252	228	157	204	258	236	226	198
281	161	754	735	756	742	758	766	705	665	789
665	277	268	315	331	315	302	274	338	337	331
267	203	164	308	313	300	314	297	152	303	284
321	193	323	282	231	273	289	382	307	241	279
334	401	198	201	226	317	385	576	98	307	123
281	295	325	264	327	358	215	370	320	230	291
316	177	271	308	227	373	241	307	356	197	397
182	443	174	263	245	126	279	222	323	267	147
357	204	283	207	217	174	264	352	330	368	52
200	346	241	324	231	390	130	333	346	382	573
235	307	371	282	304	191	738	97	419	205	358
133	354	322	320	286	906	202	387	205	127	417
216	369	308	224	174	217	393	284	358	209	299
174	284	196	309	215	353	353	175	364	297	363
324	351	198	286	544	251	179	208	243	274	376
589	580	203	337	316	297	139	293	313	258	218
176	269	310	336	330	650	540	752	427	740	331
676	606	385	298	339	746	375	350	279	313	604
311	692	647	259	315	134	305	169	314	300	299
499	571	335	359	311	400	290	334	308	230	

1813.5_1313EC199		308	323	218	272	324	260	319	285	507
243	270	336	319	312	379	379	278	276	413	390
652	307	265	331	238	281	450	345	232	455	319
429	455	459	339	424	544	283	504	287	378	298
267	221	276	421	328	270	332	315	221	278	292
391	325	374	396	395	290	322	389	283	422	290
342	268	485	346	346	288	369	235	350	347	328
250	308	999	218	342	280	377	216	315	499	438
407	419	434	414	369	418	184	429	718	438	463
425	467	432	448	285	449	245	445	191	230	536
538	243	412	413	420	280	343	212	403	274	404
360	323	194	177	362	410	363	218	223	321	314
387	272	275	245	259	252	151	272	268	291	256
253	256	187	340	355	338	340	329	344	324	404
339	354	349	288	518	546	340	498	394	545	506
507	312	284	207	482	510	513	263	320	219	359
338	309	397	328	356	296	187	351	276	385	295
286	403	341	165	190	239	319	508	294	193	327
91	296	352	439	301	352	374	734	293	287	281
274	290	173	275	326	196	424	334	266	387	202
401	168	553	193	263	364	0	217	199	402	316
254	297	110	336	261	330	271	302	218	680	412
181	276	207	334	384	196	414	242	252	388	472
445	298	331	335	293	298	208	344	111	327	270
334	146	427	381	305	646	356	172	307	261	172
459	287	694	366	246	197	325	409	512	353	212
291	541	349	152	400	205	405	446	232	455	253
451	697	477	221	637	394	278	214	261	239	641
424	280	252	279	421	380	457	244	397	369	292
224	164	257	386	432	643	403	275	344	317	320
345	531	314	326	379	394	345	415	392	205	339
377	397	410	222	554	430	157	538	247	492	522
650	288	357	341	347	319	316	348	373	316	250

1820.5_1185EK04	341	376	228	405	404	338	389	161	274	303
601	358	482	519	331	340	363	263	296	364	313
371	251	281	483	315	295	513	376	339	395	308
349	317	275	311	253	221	333	441	349	393	322
287	608	350	251	212	313	356	255	323	566	302
326	258	292	284	375	370	283	305	245	280	288
271	245	290	271	314	235	519	266	233	224	343
237	218	999	240	253	275	203	286	297	282	255
260	270	274	339	275	195	273	257	273	256	260
256	262	241	234	235	271	238	462	538	255	248
217	228	227	230	305	273	242	292	270	290	248
245	261	174	249	246	222	262	493	259	408	217
284	318	276	191	332	601	223	323	280	319	206
279	585	253	250	243	265	218	258	273	306	283
224	220	243	250	244	231	257	223	249	261	260
252	222	214	220	272	259	201	195	145	178	230
97	162	163	178	249	164	291	178	238	196	374
385	323	91	530	302	389	318	202	222	369	635
527	253	319	253	310	334	172	315	381	294	316
299	501	372	401	335	307	535	599	302	101	316
303	289	293	254	380	249	252	406	361	300	210
245	0	243	479	658	357	322	478	221	301	116
324	75	393	297	377	301	275	389	270	258	310
251	229	298	336	331	697	267	337	229	349	223
393	296	316	104	217	236	903	216	284	315	345
223	185	290	219	615	155	247	219	230	197	270
1	235	134	251	514	304	223	184	238	322	336
179	253	640	263	253	283	482	270	523	243	202
270	20	522	295	221	445	395	450	427	280	288
216	258	437	276	203	218	186	199	187	205	350
232	178	246	332	321	277	340	250	17	261	251
279	232	144	262	263	211	249	161	284	290	220
261	229	306	314	301	310	219	298	277	227	

1821.6_1288EC03	250	268	157	292	290	244	304	273	414	241
220	285	231	320	493	374	282	482	432	329	293
350	242	344	237	257	398	263	230	352	257	362
360	376	466	433	444	210	412	288	237	254	302
256	284	400	250	176	367	325	218	268	264	360
231	343	375	380	212	273	385	358	407	297	320
348	415	352	311	305	380	280	323	514	344	330
364	342	240	999	280	793	185	424	397	427	374
386	406	373	242	420	141	480	436	470	480	389
491	469	449	237	430	188	430	217	265	474	480
269	497	490	460	217	412	211	390	258	393	447
377	235	191	472	461	364	239	217	248	370	452
287	270	254	256	250	179	218	313	210	257	273
273	199	351	402	379	388	374	421	383	461	371
402	424	384	459	473	405	451	416	462	461	457
368	250	281	474	461	483	239	298	153	313	320
313	337	303	302	248	251	309	299	410	264	275
385	345	142	225	229	304	426	234	135	289	117
223	376	347	265	542	324	311	435	346	313	259
291	165	308	318	190	395	274	276	464	153	438
184	478	181	261	235	109	263	229	350	259	153
458	0	476	226	273	291	245	299	440	404	42
249	117	297	386	316	445	241	326	399	440	457
291	409	234	288	311	211	414	141	385	345	388
146	380	459	315	413	351	212	773	195	203	460
284	518	414	296	176	243	397	314	354	187	417
366	473	75	468	225	414	482	180	493	253	431
460	464	235	438	315	264	234	327	257	460	474
331	141	298	489	483	381	171	393	371	275	253
157	316	333	370	441	413	268	381	383	401	400
397	372	419	429	387	424	406	457	272	391	392
400	402	207	404	448	159	424	248	464	446	453
266	364	381	389	360	359	284	364	319	373	

1821.6_2011EC49	340	329	162	279	279	289	299	247	447	185
232	314	301	354	439	461	246	245	464	318	282
364	230	394	282	219	368	314	321	472	306	438
462	472	339	437	411	200	381	267	312	322	271
251	278	451	267	230	378	296	277	254	246	476
371	335	355	347	314	258	352	265	346	244	363
254	375	380	367	242	325	247	365	345	282	241
257	280	253	280	999	389	226	306	345	387	306
315	361	337	336	342	192	401	353	399	313	357
338	398	382	209	403	225	400	225	238	371	390
516	341	340	351	338	317	208	367	632	368	353
300	273	398	390	366	323	329	225	387	285	351
509	348	228	467	300	199	211	288	240	197	195
373	226	302	308	322	331	293	339	335	397	328
324	288	241	320	287	353	279	252	344	319	358
275	239	207	285	292	309	250	402	220	438	407
410	352	424	419	213	328	371	458	272	236	296
394	508	221	207	262	299	437	235	162	336	93
259	436	427	257	363	278	274	375	399	283	228
379	183	284	347	215	448	283	253	386	253	414
152	394	187	209	308	109	278	212	363	298	261
325	160	273	226	278	244	363	273	323	344	55
274	215	273	335	308	365	186	313	362	369	374
211	354	258	278	261	258	325	163	272	275	322
150	361	313	257	280	285	162	290	270	134	323
198	330	327	213	221	263	322	231	292	251	287
174	309	202	329	231	419	351	193	363	332	339
281	390	229	283	270	245	174	238	203	290	353
299	179	270	375	302	322	116	340	337	284	225
220	241	326	353	337	305	303	282	259	332	334
231	311	246	289	269	349	424	242	275	356	243
246	303	210	267	278	161	285	213	271	265	262
245	256	321	324	336	384	359	382	348	206	

1826.9_1313EC200		312	331	237	314	297	294	327	342	451
264	307	302	303	412	459	480	304	401	467	328
370	393	288	409	299	333	481	355	296	394	321
366	405	398	458	470	485	289	496	353	342	324
368	305	357	431	293	203	440	332	324	321	308
423	286	346	394	395	294	362	390	402	450	384
318	387	458	346	324	405	429	285	337	513	457
301	414	377	275	793	389	999	301	347	429	438
382	396	423	416	320	424	234	418	481	411	485
435	499	411	381	343	416	285	390	249	316	496
507	415	428	432	456	275	401	243	453	364	450
462	392	277	214	461	470	401	405	256	330	398
453	399	377	340	252	311	273	307	312	253	268
299	407	281	360	389	375	372	342	402	368	536
414	434	429	392	443	446	425	441	418	437	446
426	398	302	292	457	451	472	281	375	234	362
385	382	387	358	341	332	308	446	356	445	345
326	449	424	202	239	267	327	462	323	198	320
173	279	452	416	347	468	330	367	468	413	337
299	317	265	304	351	240	490	384	347	474	198
482	247	547	233	305	349	144	317	276	442	322
188	489	118	548	312	358	327	311	388	482	430
194	321	181	390	475	381	536	278	400	379	488
485	438	474	300	378	359	292	455	272	411	356
417	156	434	493	377	437	413	266	955	382	239
502	327	497	408	332	251	331	421	323	403	287
430	266	384	222	420	316	457	438	246	461	315
498	475	491	294	464	427	388	315	377	303	479
491	419	314	331	454	424	419	211	435	390	405
362	240	369	391	448	465	453	348	384	372	415
413	427	426	441	470	437	396	530	474	336	466
507	425	393	244	412	460	214	484	305	459	494
417	384	428	548	552	512	530	398	497	486	484

1843.5_2011EC47	210	294	187	195	196	219	205	184	225	129	
	195	210	194	216	174	208	191	184	200	275	221
	270	199	298	208	173	192	191	220	209	240	193
	215	185	195	232	248	220	240	226	187	260	179
	197	184	215	248	222	285	204	609	237	189	197
	364	216	179	181	205	182	183	278	197	197	166
	234	216	215	174	188	265	194	197	176	204	180
	201	216	203	185	226	301	999	152	248	253	190
	187	190	189	156	189	313	184	208	184	213	203
	215	179	171	211	182	352	191	209	199	225	253
	283	188	189	205	239	170	207	208	268	207	175
	160	198	222	173	177	160	255	170	325	248	234
	261	337	297	238	217	224	198	200	254	219	182
	292	203	206	292	229	241	240	281	290	349	259
	230	167	185	168	169	338	174	188	227	244	225
	316	187	235	178	183	188	243	232	50	243	257
	197	93	238	171	181	118	312	248	202	169	190
	251	268	244	135	214	205	215	166	120	224	102
	159	69	259	177	215	170	171	211	283	139	215
	167	214	202	205	230	199	221	246	153	127	184
	176	240	169	127	210	205	184	169	199	231	215
	199	264	216	160	248	184	368	192	189	202	37
	235	96	201	167	219	205	196	205	180	209	272
	203	120	209	208	181	217	173	148	191	209	115
	155	222	136	163	230	174	193	198	361	155	231
	204	175	210	231	208	226	188	162	189	240	215
	139	140	281	178	204	209	187	208	197	228	214
	185	190	214	204	196	301	199	242	191	185	189
	180	6	101	240	174	161	147	144	181	323	269
	184	243	183	238	204	165	258	130	194	202	146
	147	193	187	218	205	254	291	198	188	188	173
	151	220	86	161	214	161	162	194	181	161	184
	199	140	314	318	269	338	288	303	285	229	

1853.9_1164EK02	287	273	166	175	196	288	335	275	410	233
211	235	344	379	395	446	292	477	341	318	247
298	289	337	339	233	383	354	259	355	307	365
350	361	339	364	384	216	382	367	259	276	222
266	357	386	215	198	351	326	197	202	354	347
262	351	353	342	259	318	337	282	412	293	279
269	419	334	286	263	303	322	286	322	370	358
331	315	286	424	306	347	152	999	342	399	403
428	408	423	215	412	220	439	444	441	448	385
433	426	394	216	398	140	409	258	368	411	417
197	418	414	397	226	301	219	386	233	385	394
306	185	217	413	374	340	212	267	194	396	350
230	291	218	235	257	307	191	239	198	197	272
203	321	323	402	307	317	308	323	342	370	351
343	379	296	411	395	339	362	341	360	350	382
325	210	287	340	378	385	191	267	292	221	270
280	207	211	264	194	280	312	314	353	216	236
396	355	157	332	289	335	411	330	265	264	229
333	415	375	255	473	290	193	368	351	331	379
319	254	277	369	227	304	277	322	364	17	361
161	448	132	260	309	32	261	323	384	246	125
404	0	408	226	284	333	289	341	340	390	160
277	121	338	374	201	419	431	301	389	442	453
337	331	288	315	390	302	400	278	322	396	386
243	396	343	271	306	317	266	282	182	349	515
213	355	492	266	303	185	439	265	429	151	489
0	397	200	445	333	395	416	187	427	280	426
332	364	287	364	267	273	245	327	264	372	328
355	308	344	469	442	453	306	404	450	280	327
117	313	394	343	343	408	217	326	328	339	389
369	337	393	457	445	418	433	410	264	375	381
355	406	249	325	402	183	369	133	374	397	344
258	356	313	354	286	366	220	345	318	325	

1854.9_1164EK03	318	303	186	289	278	290	330	257	478	250
257	258	304	351	465	450	288	379	427	347	370
352	274	356	251	454	389	299	278	410	271	401
405	395	369	466	519	247	497	290	276	249	293
298	319	422	276	273	289	268	275	256	255	389
295	435	458	463	251	301	452	282	469	285	359
263	482	378	366	275	330	222	361	354	325	282
331	499	297	397	345	429	248	342	999	417	425
433	403	431	316	448	186	470	532	461	501	426
502	452	444	304	451	228	448	173	257	515	500
270	451	455	467	276	380	165	382	282	382	435
397	212	173	478	465	428	273	221	295	318	488
303	293	274	226	278	197	310	320	242	234	295
298	196	304	375	297	319	302	344	313	483	346
444	381	331	479	486	328	468	447	481	503	497
350	336	294	588	456	460	253	666	489	379	671
324	400	410	564	329	256	374	265	462	330	295
401	353	139	197	272	330	476	243	225	296	153
286	423	395	414	439	364	402	376	350	346	281
317	207	298	337	186	452	356	294	448	213	465
168	514	247	288	298	30	304	225	377	285	229
429	6	423	263	319	226	303	292	524	445	164
270	174	320	444	290	479	220	371	455	497	463
320	375	319	334	325	254	329	298	456	314	436
236	401	489	409	521	308	230	383	272	233	484
302	594	426	288	219	290	445	379	428	204	408
325	381	201	425	245	462	456	271	466	298	457
569	512	241	461	370	292	266	361	279	472	538
353	222	331	452	450	563	230	469	528	285	256
184	338	385	370	474	418	297	340	392	337	413
375	354	462	450	436	335	459	481	264	441	440
479	404	193	463	507	203	479	244	488	480	493
351	401	370	399	375	378	382	403	333	369	

1862.2_2011EC39	277	297	201	304	303	296	315	287	611	246	
	277	305	312	377	431	429	309	344	381	351	338
	445	247	477	310	271	424	333	311	497	402	492
	505	492	443	466	738	248	629	416	333	293	306
	313	352	510	287	236	388	335	265	310	292	463
	320	643	642	637	300	291	633	335	648	301	428
	318	680	447	437	330	326	255	449	372	332	284
	328	438	282	427	387	438	253	399	417	999	681
	693	976	687	364	675	206	544	550	545	661	971
	662	524	530	204	547	241	537	223	288	619	620
	332	550	561	649	328	372	244	439	326	444	466
	394	304	278	575	541	382	334	254	331	387	517
	342	360	240	291	296	321	191	338	278	300	205
	334	267	342	438	356	336	349	388	364	451	346
	420	461	431	550	546	413	500	441	645	529	627
	431	207	296	537	452	472	202	389	301	415	402
	446	335	423	415	197	338	404	446	409	221	332
	370	434	167	238	267	315	624	297	244	314	184
	294	397	464	319	391	386	310	413	468	261	303
	253	237	266	334	328	353	282	308	448	145	474
	198	702	175	292	347	211	291	278	489	302	215
	431	118	477	339	334	289	363	327	673	647	227
	325	200	362	445	318	623	268	412	552	700	457
	384	325	293	307	399	307	359	299	572	307	578
	187	531	528	442	478	295	271	356	347	234	592
	285	584	535	322	251	335	736	340	716	260	544
	334	497	197	530	290	361	617	258	633	375	616
	543	564	235	556	308	334	316	322	287	527	526
	408	307	326	538	551	586	372	445	573	384	354
	261	332	607	569	524	500	275	340	510	365	589
	373	360	524	555	543	431	498	511	379	515	434
	471	379	221	442	493	147	477	253	467	489	505
	332	396	367	425	359	422	320	454	403	363	

1865.3_1135EC00 276 272 118 296 296 302 253 252 635 247
268 300 280 364 370 406 284 306 398 313 320
424 250 477 298 262 387 310 323 507 420 482
495 484 396 478 832 181 730 360 265 255 264
263 320 537 298 204 275 251 243 284 230 477
316 887 898 902 244 319 888 312 834 264 424
302 797 434 430 257 357 234 457 336 336 258
384 407 255 374 306 382 190 403 425 681 999
975 709 942 306 908 159 590 593 610 772 680
771 572 587 129 613 112 612 203 229 716 719
291 667 682 804 344 438 182 419 301 427 453
451 197 275 617 589 392 248 218 259 378 573
319 321 204 300 307 235 118 338 235 235 128
285 233 385 465 397 372 412 437 407 425 370
465 579 405 580 583 384 558 519 721 576 717
415 143 283 603 529 543 167 378 255 439 383
381 369 404 449 152 300 324 430 491 179 327
396 337 135 195 274 253 646 264 232 313 173
303 371 510 218 342 345 305 428 450 247 286
230 221 241 342 324 362 266 286 381 185 484
139 782 225 223 294 60 241 247 499 293 194
377 0 401 226 292 217 332 290 636 915 33
231 172 364 436 271 724 243 442 565 806 507
347 348 202 254 460 236 374 175 646 277 705
172 560 552 457 494 278 247 385 221 166 614
227 610 581 301 200 319 966 353 921 147 586
392 528 131 573 222 383 688 183 703 379 705
561 621 225 527 353 249 258 298 223 495 545
457 338 316 556 614 626 428 458 634 270 284
247 294 597 476 552 547 265 368 637 436 597
404 360 583 579 527 458 438 608 338 524 409
521 453 246 380 571 139 475 229 541 539 512
229 420 279 338 296 366 239 371 295 301

1866.7_1185EK18	287	299	180	306	306	311	259	267	628	245
263	310	285	383	376	453	290	330	384	329	328
431	252	488	296	265	387	320	334	518	432	495
506	498	389	512	825	216	727	387	275	259	278
292	315	546	310	219	301	268	248	296	234	480
343	882	894	897	254	321	883	321	819	277	427
319	791	441	435	260	341	243	465	329	340	267
388	419	260	386	315	396	187	428	433	693	975
999	724	941	303	933	160	594	593	615	785	690
771	578	591	160	618	180	621	195	241	693	694
285	653	667	788	357	443	171	426	303	432	478
454	202	281	640	608	426	237	199	284	379	572
322	345	213	299	289	249	151	322	233	241	175
269	210	388	485	402	377	414	445	406	434	377
473	580	406	577	579	393	557	517	701	572	711
427	172	305	591	529	537	218	377	256	433	383
372	374	400	439	197	317	321	430	488	201	331
404	361	176	181	280	259	643	277	236	324	158
299	424	520	243	342	349	297	378	453	259	283
238	181	261	356	332	366	280	310	388	206	518
142	781	193	260	298	26	256	281	491	313	200
360	0	414	228	298	240	339	311	641	911	39
276	175	371	443	277	717	246	446	595	799	525
333	349	229	254	449	220	380	124	640	273	701
158	565	578	465	483	285	243	391	216	141	625
231	605	567	318	212	379	960	349	930	186	586
375	521	136	574	230	396	685	200	697	392	704
556	635	197	526	314	296	242	334	230	495	550
458	342	314	555	621	627	431	479	646	322	336
237	328	637	469	545	569	288	372	631	443	603
404	344	590	564	532	477	461	609	333	530	414
519	446	243	381	565	88	476	208	542	543	524
229	441	293	357	320	361	255	375	279	327	

1869.2_1344EC16	300	291	140	311	311	295	326	240	655	208	
	268	310	302	381	434	489	319	323	404	375	337
	433	259	491	309	262	420	321	318	538	410	527
	524	515	381	464	759	157	655	421	306	275	291
	323	329	490	291	219	390	289	226	308	255	447
	328	692	693	691	289	278	687	289	684	265	425
	298	723	452	434	254	281	259	457	367	374	278
	323	434	270	406	361	423	190	408	403	976	709
	724	999	712	374	726	159	575	553	572	675	975
	675	553	583	115	598	125	593	200	252	632	632
	314	545	555	658	321	363	228	443	269	444	420
	396	269	251	545	500	353	227	219	280	372	525
	301	324	246	277	267	298	107	304	265	284	163
	249	262	379	486	387	377	408	454	417	440	312
	433	495	414	540	549	394	528	477	672	553	666
	381	112	291	526	484	497	158	379	271	411	397
	407	335	398	437	119	324	332	415	438	134	335
	387	440	148	212	268	326	659	254	190	334	151
	294	451	483	256	352	397	294	403	453	249	307
	280	191	240	350	314	386	266	311	415	138	478
	204	726	128	292	326	27	289	296	476	307	193
	400	0	444	306	306	240	338	291	683	697	246
	269	145	340	425	277	677	236	404	596	726	489
	361	348	257	295	379	273	400	159	615	293	634
	158	549	527	492	466	283	217	429	229	199	578
	271	582	510	303	226	318	762	322	740	150	512
	318	483	152	507	243	437	631	177	654	356	627
	536	576	212	505	284	257	305	335	263	449	526
	420	263	313	516	541	567	388	443	586	286	265
	230	331	610	528	515	515	268	339	543	395	619
	401	419	551	518	503	467	485	564	306	507	369
	506	346	237	463	513	101	482	226	500	516	497
	263	411	290	346	310	389	247	388	313	307	

1870.1_1135EC00	288	279	134	332	325	296	290	229	625	235
275	310	311	378	401	430	303	312	420	340	326
437	256	473	311	248	397	340	324	510	452	479
496	485	405	502	822	173	719	373	310	266	300
288	326	551	325	192	342	283	218	346	253	492
329	885	911	909	296	336	900	320	803	253	432
309	812	443	439	240	342	264	461	341	333	269
373	414	274	373	337	416	189	423	431	687	942
941	712	999	280	964	147	601	595	619	781	687
764	585	604	149	637	125	620	218	253	682	686
289	634	647	807	353	467	181	448	324	455	460
413	204	293	608	582	404	269	213	287	390	575
340	334	246	315	312	249	133	357	244	254	133
289	234	415	494	434	406	417	452	419	450	398
445	554	425	547	557	407	555	500	737	569	733
442	147	262	603	519	530	181	393	312	503	399
454	440	473	525	157	362	319	506	469	161	361
411	357	105	221	290	290	639	248	204	334	149
294	423	503	227	354	366	319	406	455	239	293
265	240	237	348	368	382	268	318	364	156	505
205	799	180	244	278	62	258	251	500	332	195
397	0	395	229	300	214	352	321	625	906	118
242	168	381	396	290	703	220	433	576	818	521
347	354	217	249	439	247	365	171	608	266	661
184	532	591	466	503	293	229	408	236	174	626
216	626	558	285	212	295	945	344	954	164	595
392	496	149	533	225	372	695	198	717	380	683
587	620	246	541	321	255	284	285	226	511	564
447	256	325	553	572	633	405	487	655	265	278
237	281	627	456	550	584	273	389	613	448	613
416	343	586	588	545	472	436	607	320	536	408
497	452	243	394	550	140	482	220	532	533	553
260	453	266	342	298	381	219	358	298	308	

1871.6_1164EK04	312	246	3	267	273	260	292	148	296	229
219	285	387	302	349	412	340	203	363	709	439
331	120	292	362	265	328	411	346	316	350	358
341	338	324	364	311	2	292	303	466	353	290
240	350	367	307	142	364	329	174	290	329	336
269	223	249	239	329	563	226	202	286	170	291
217	309	211	293	153	204	338	225	308	207	371
201	369	339	242	336	320	156	215	316	364	306
303	374	280	999	284	103	294	279	297	229	363
234	277	255	3	257	156	261	177	343	252	255
195	278	278	299	287	322	281	306	149	308	269
232	317	180	237	276	246	137	247	244	380	218
158	244	228	239	392	319	5	395	360	372	124
172	253	206	241	207	209	203	242	283	291	185
265	247	286	254	240	220	275	234	259	256	282
248	3	131	215	251	233	153	319	131	263	291
275	220	293	269	7	129	226	262	197	3	262
462	407	1	255	308	292	278	92	243	327	44
321	380	339	296	243	655	275	224	313	232	220
342	62	274	330	308	352	288	319	362	207	347
359	305	188	515	469	0	229	236	332	260	146
276	0	246	234	336	287	302	378	362	284	151
103	43	564	286	276	228	272	322	313	319	301
229	317	235	242	244	303	277	78	277	369	265
127	304	262	308	276	242	264	351	107	106	308
179	336	235	195	269	281	302	178	280	1	224
29	215	1	312	311	342	310	247	318	366	325
309	332	301	343	218	105	259	101	323	365	235
252	153	334	294	287	336	121	308	323	146	149
311	102	348	325	332	257	159	231	219	214	294
286	273	226	321	288	275	320	258	129	279	200
258	200	5	340	242	208	288	5	264	290	296
176	238	175	174	177	222	214	213	176	189	

1875.4_1185EK18	294	325	146	303	289	300	278	269	625	256
272	313	302	395	380	445	292	310	407	348	348
425	242	490	332	259	426	345	349	539	454	515
541	535	410	490	805	180	712	407	300	299	291
306	333	544	302	220	354	284	237	319	262	477
328	841	872	869	280	327	858	336	822	277	418
329	789	429	428	250	376	264	456	383	322	302
374	418	275	420	342	424	189	412	448	675	908
933	726	964	284	999	175	603	608	620	774	698
752	586	601	126	628	102	627	213	256	696	699
294	615	627	784	344	453	185	473	297	480	490
457	246	235	645	612	417	223	181	273	388	573
311	356	237	262	313	257	118	355	235	243	130
258	245	403	498	418	395	420	439	401	448	393
482	553	428	576	584	416	571	511	731	577	744
422	122	258	583	530	536	197	378	251	425	378
347	360	404	448	132	307	304	415	469	145	333
415	361	172	209	274	278	642	269	245	356	156
309	432	505	237	364	368	302	420	457	247	293
279	198	245	372	345	374	291	331	422	176	498
182	786	237	282	319	26	271	286	493	304	204
431	0	402	246	307	254	320	328	639	889	144
274	198	372	450	306	738	227	435	577	797	541
347	375	245	273	440	237	379	144	694	310	677
171	552	571	447	486	278	245	425	222	171	636
233	615	554	289	234	295	910	348	952	137	591
386	490	138	528	241	422	690	183	704	375	691
564	673	240	527	331	249	238	284	242	498	559
450	337	312	562	576	633	427	484	677	295	302
219	278	680	451	551	597	273	381	613	451	622
423	376	597	573	521	485	463	611	322	536	421
519	465	268	383	553	92	477	261	543	552	527
257	461	284	344	294	363	247	373	272	310	

1879.6_1344EC04 227 237 284 189 186 218 203 166 152 163

207	209	227	213	250	209	213	237	145	208	188
215	179	184	210	197	154	242	282	167	250	137
168	155	167	225	154	318	201	210	187	255	227
193	213	129	225	131	234	220	261	139	238	218
231	154	161	144	268	212	149	219	112	175	171
175	142	193	178	172	226	197	188	205	152	205
182	184	195	141	192	234	313	220	186	206	159
160	159	147	103	175	999	114	154	115	163	148
176	137	134	294	144	351	141	243	197	160	176
230	111	111	113	261	140	166	140	230	127	125
185	181	175	139	129	159	255	153	275	240	191
281	226	328	208	189	261	299	201	223	47	182
288	213	194	204	216	212	203	242	232	265	236
219	179	170	158	161	364	147	208	178	186	187
298	288	215	144	138	137	233	143	155	135	238
186	89	218	130	297	154	268	225	185	287	217
217	179	172	175	223	203	131	190	210	233	273
209	138	141	253	159	165	95	127	206	161	257
126	175	225	164	240	236	275	238	178	192	182
66	166	160	181	176	233	195	221	143	221	109
213	170	156	196	214	188	276	161	139	156	24
182	103	220	143	130	123	221	170	127	107	219
215	145	190	287	129	231	110	55	143	240	106
124	163	115	164	178	71	215	107	376	246	188
136	169	167	202	248	153	124	137	131	676	190
129	169	223	146	257	140	122	197	117	239	150
164	146	236	157	85	294	269	222	208	144	209
155	196	122	181	103	124	94	128	146	333	303
144	222	144	199	141	163	258	183	208	135	141
129	147	198	141	165	198	245	156	141	159	146
183	179	50	123	233	215	113	259	149	129	150
247	92	279	306	245	231	289	253	254	209	

1879.8_1185EK17	309	322	194	335	322	305	355	251	653	292	
285	345	320	371	416	456	335	339	400	367	379	
434	259	476	279	273	442	330	306	640	376	627	
654	662	410	477	678	254	617	356	377	324	342	
333	322	549	338	196	347	339	206	276	318	455	
324	609	616	619	298	303	608	303	724	299	483	
309	756	539	483	298	333	286	508	380	364	285	
317	429	273	480	401	418	184	439	470	544	590	
594	575	601	294	603	114	999	584	970	641	555	
660	982	969	242	905	156	940	218	292	643	642	
313	812	801	758	323	434	240	529	268	511	579	
413	345	244	665	634	340	272	203	311	396	529	
325	369	269	284	303	248	209	309	292	260	233	
277	269	446	493	461	441	463	465	441	452	382	
439	519	342	680	668	366	648	466	629	636	623	
359	248	337	597	601	599	207	360	190	342	369	
341	309	335	371	258	187	330	396	468	277	350	
417	476	171	208	305	355	671	233	273	360	129	
297	447	476	231	393	349	342	406	416	257	281	
389	202	423	483	264	418	306	317	397	200	468	
237	709	150	255	324	23	323	247	532	286	223	
396	0	408	230	342	261	317	337	611	619	28	
314	124	355	396	304	658	257	390	542	759	476	
349	378	268	259	421	206	378	106	530	296	506	
184	510	605	440	527	283	198	409	268	204	591	
305	584	679	338	218	316	600	349	575	109	690	
346	921	161	915	254	428	839	245	838	340	630	
563	654	244	702	311	306	264	358	245	697	556	
459	214	301	778	847	672	342	491	560	327	350	
217	356	521	516	559	501	320	440	491	485	617	
421	397	488	520	482	475	474	546	257	458	411	
470	448	243	511	526	148	576	180	604	591	581	
269	417	314	388	281	372	244	395	316	350		

1879.9_1344EC77	315	353	157	326	341	332	305	273	647	232
295	382	331	326	389	414	274	360	401	401	561
405	260	450	279	245	476	377	315	503	427	471
516	531	432	486	714	193	643	386	403	303	344
276	307	546	353	218	417	374	257	297	346	446
351	522	521	518	297	387	517	360	631	307	455
357	664	473	462	280	364	307	474	333	385	298
384	718	257	436	353	481	208	444	532	550	593
593	553	595	279	608	154	584	999	601	646	537
648	589	621	211	615	177	606	245	315	669	669
328	561	567	592	314	464	271	485	336	490	500
447	260	279	541	546	424	286	258	354	387	507
327	362	241	319	275	170	223	268	338	303	255
305	209	417	472	433	409	432	470	425	461	432
449	500	417	663	691	407	625	513	676	632	658
441	235	280	605	636	643	239	406	218	384	398
369	375	357	400	243	228	352	398	511	253	342
432	426	153	177	306	305	658	244	144	400	150
294	405	462	246	394	330	558	423	381	317	269
295	140	297	401	300	414	305	369	428	274	494
268	738	105	265	340	13	277	264	504	323	283
410	0	409	287	398	301	345	307	695	581	109
230	197	402	395	318	609	197	360	492	690	563
355	305	290	265	425	230	421	124	510	303	515
140	502	600	357	716	359	234	394	203	196	605
295	803	574	303	194	229	605	746	546	144	491
469	515	187	545	253	479	621	187	634	356	653
800	611	233	756	393	280	198	350	283	753	575
399	134	253	558	556	638	341	478	586	317	251
236	350	560	499	752	568	252	409	486	427	503
571	378	522	487	490	510	502	559	259	452	426
518	488	163	533	560	136	686	184	651	663	747
347	456	335	345	331	389	243	395	320	291	

1883.7_1185EK19	318	328	188	347	333	301	340	229	656	286
293	355	325	376	409	470	336	340	406	373	378
449	254	490	290	276	429	348	326	638	382	628
652	663	405	475	707	245	640	354	362	315	342
342	315	525	325	197	346	345	202	283	311	461
345	650	654	653	292	289	643	297	743	288	468
301	778	526	469	284	327	299	495	376	352	301
306	438	273	470	399	411	184	441	461	545	610
615	572	619	297	620	115	970	601	999	662	557
682	972	955	243	928	188	934	221	281	658	658
295	841	830	787	345	424	216	506	271	488	583
402	344	251	673	636	330	274	203	311	393	556
330	373	273	292	322	254	218	333	278	270	251
278	285	439	494	455	442	464	459	451	447	381
446	516	341	693	682	368	648	463	641	641	638
356	273	341	613	599	607	218	358	240	366	361
379	364	354	393	282	278	329	443	459	304	363
418	466	173	208	295	340	675	229	271	367	130
301	466	472	245	399	357	354	409	436	261	285
384	203	415	474	288	416	309	319	390	201	467
232	711	148	262	314	20	332	249	512	294	202
397	0	426	237	335	253	350	356	623	638	24
317	118	344	398	303	656	253	397	549	794	482
358	377	276	279	416	207	361	116	532	293	509
184	492	598	452	539	285	198	404	269	202	593
292	602	674	330	220	341	640	360	610	153	696
364	920	169	903	256	429	866	243	861	353	640
573	658	246	681	300	319	266	363	236	672	594
471	225	330	797	858	667	317	506	556	329	357
201	360	523	502	578	507	320	433	508	482	640
410	397	509	512	478	480	478	553	265	471	400
475	451	236	517	521	151	583	188	605	588	590
258	407	315	396	290	368	270	397	314	343	

1884.8_2011EC37	272	281	140	346	310	288	326	246	627	252	
	250	364	278	356	417	394	269	442	416	361	393
	465	266	491	286	251	446	325	358	497	429	460
	487	466	488	545	838	178	740	384	357	285	384
	240	315	674	353	186	358	350	245	255	298	614
	337	684	699	700	286	348	692	334	803	307	439
	330	800	480	445	271	443	279	464	332	363	306
	404	463	256	480	313	485	213	448	501	661	772
	785	675	781	229	774	163	641	646	662	999	654
	993	638	649	184	680	198	655	257	273	885	885
	319	635	645	761	377	518	256	453	356	462	568
	499	208	284	702	669	538	300	251	371	452	633
	375	378	253	350	328	176	202	356	265	269	240
	336	206	417	514	433	416	430	477	421	470	466
	485	630	518	650	664	494	622	592	732	620	735
	502	233	317	646	597	615	206	414	181	433	425
	388	368	403	436	224	276	418	434	587	265	355
	454	407	177	253	272	326	657	240	175	366	141
	256	411	534	246	503	343	401	424	463	370	266
	293	202	258	326	335	384	330	336	402	217	539
	189	792	191	313	318	117	242	252	605	358	191
	462	0	490	273	364	319	370	319	609	760	212
	243	157	404	509	324	710	204	487	617	819	600
	340	323	227	280	423	227	369	182	691	333	730
	166	531	668	443	614	295	237	421	251	179	668
	303	718	629	304	173	231	790	437	744	155	630
	313	544	173	571	242	446	718	186	730	390	793
	656	711	215	596	356	285	189	336	285	589	686
	467	179	366	608	597	673	390	537	634	317	293
	210	313	602	517	650	601	296	431	688	452	563
	476	380	711	584	581	513	495	723	411	532	479
	625	490	210	441	655	181	594	226	630	631	680
	380	536	358	394	371	385	285	420	335	338	

1886.0_1344EC16	284	278	169	305	306	295	314	234	635	209
277	299	297	388	425	460	314	332	388	358	335
441	251	479	301	241	411	321	291	525	393	517
514	502	391	457	751	166	632	421	303	271	287
319	339	504	287	211	386	282	225	298	250	450
325	668	672	669	279	268	664	299	663	259	432
282	684	459	442	243	271	268	458	358	349	265
334	425	260	389	357	435	203	385	426	971	680
690	975	687	363	698	148	555	537	557	654	999
654	535	554	127	576	168	567	205	248	602	601
310	523	534	636	323	382	218	429	268	435	426
371	270	261	534	512	358	226	211	285	391	516
295	325	242	278	255	296	115	321	274	289	169
242	258	379	476	399	382	406	438	399	432	334
445	483	425	535	542	396	517	467	662	535	659
403	122	291	517	474	484	207	386	257	431	399
413	349	413	451	147	319	335	432	427	141	330
355	442	136	214	267	314	642	244	193	317	156
293	437	464	253	356	383	300	388	460	246	294
268	194	232	331	301	353	268	321	406	140	467
204	712	162	278	322	28	301	283	496	302	186
419	0	523	333	304	240	337	312	665	671	247
271	189	330	451	271	636	224	396	593	696	484
354	342	276	310	397	272	385	171	609	267	579
150	550	538	501	452	275	255	350	225	208	571
201	574	496	288	229	336	737	317	722	188	518
317	471	146	513	237	429	604	183	626	358	612
532	569	208	524	311	250	302	311	260	490	517
405	242	311	500	520	560	379	458	583	303	290
243	310	613	536	509	527	258	355	531	404	595
387	404	528	524	519	466	462	551	293	491	378
496	371	248	459	499	100	481	219	490	501	489
276	421	274	329	294	369	260	363	290	308	

1886.5_2011EC38	280	296	188	347	312	291	320	246	625	236
252	357	275	369	401	394	254	446	415	357	404
471	268	490	287	267	448	334	364	501	430	468
489	472	489	546	838	229	743	388	358	290	380
253	321	676	358	187	379	354	257	277	298	616
334	709	713	718	279	351	709	327	802	299	434
328	801	476	440	253	435	282	458	333	363	308
405	467	256	491	338	499	215	433	502	662	771
771	675	764	234	752	176	660	648	682	993	654
999	660	670	210	702	206	678	259	288	887	888
316	635	645	759	372	535	255	453	358	462	576
516	208	282	703	670	541	287	250	382	460	630
344	388	254	351	324	186	227	374	267	273	248
330	212	435	512	452	435	449	496	440	471	467
485	630	524	665	679	490	637	590	733	632	725
507	264	318	651	609	625	219	416	167	434	426
396	370	404	437	265	278	411	434	596	306	356
464	409	162	227	276	320	655	242	146	362	139
267	411	541	269	505	351	403	424	469	375	290
307	228	259	329	335	387	343	349	402	285	538
188	794	191	312	320	107	263	235	620	357	184
461	2	487	271	371	322	367	339	608	795	154
273	165	405	516	342	707	187	484	609	819	600
333	351	199	296	429	236	370	215	691	345	732
174	523	668	443	615	297	242	439	265	184	671
290	715	620	309	186	240	788	438	721	170	636
308	551	171	576	257	426	718	210	731	385	792
651	713	213	601	350	313	197	353	290	595	681
472	179	366	606	597	655	390	521	620	333	303
214	334	588	513	654	589	309	455	672	477	565
478	381	716	584	587	514	500	721	405	533	479
626	489	242	469	651	175	594	228	642	642	680
386	562	354	403	390	386	277	430	329	355	

1889.8_1185EK16	296	313	199	318	307	282	331	230	656	273
274	315	310	376	423	495	326	327	396	366	347
421	258	494	274	272	436	350	290	646	362	632
660	668	407	475	681	265	622	342	351	305	324
316	316	533	307	199	333	340	193	264	291	453
330	604	622	617	279	286	606	285	724	276	469
290	752	527	469	276	321	297	492	380	335	299
303	432	262	469	398	411	179	426	452	524	572
578	553	585	277	586	137	982	589	972	638	535
660	999	965	228	899	143	935	221	267	639	639
283	813	802	757	326	430	188	500	255	482	575
389	339	227	659	622	325	269	203	304	388	549
311	366	251	261	282	255	205	309	263	287	212
278	270	434	479	447	438	457	450	440	443	358
438	506	312	687	671	353	641	451	633	635	623
339	242	340	599	594	602	206	332	193	330	338
324	311	319	339	262	198	322	369	454	272	337
421	451	150	211	274	331	673	247	278	347	131
306	435	468	234	385	344	317	401	423	264	283
398	205	412	489	268	428	299	303	403	208	474
209	693	149	265	316	24	306	235	525	271	194
394	0	407	213	324	240	328	328	609	620	28
301	117	342	394	291	641	263	388	536	768	469
348	379	247	238	406	196	361	109	510	293	498
186	491	573	449	529	289	198	402	256	209	586
231	587	679	342	217	290	586	359	576	95	693
244	923	157	909	241	428	839	224	834	335	631
567	644	235	703	308	302	273	360	229	699	571
465	224	324	780	846	654	311	498	542	309	358
211	345	491	478	560	482	310	429	486	473	621
407	396	493	509	472	499	464	540	278	462	390
461	431	244	519	516	157	586	184	599	583	583
257	402	302	392	278	366	253	392	315	351	

1894.9_1185EK17	285	328	187	310	273	275	299	216	681	249
232	327	310	367	382	481	289	309	410	377	370
404	242	484	257	249	429	353	285	660	359	663
668	682	387	441	711	227	637	333	316	290	311
301	274	545	320	210	325	332	190	256	268	436
327	630	636	633	248	285	624	255	748	272	462
264	785	514	456	263	336	301	487	369	333	271
292	448	241	449	382	381	171	394	444	530	587
591	583	604	255	601	134	969	621	955	649	554
670	965	999	169	929	160	982	199	247	642	640
267	823	812	768	319	427	193	501	241	481	536
373	331	196	637	605	323	266	192	284	367	537
292	375	227	234	266	253	161	326	251	259	223
276	261	431	466	443	419	448	459	450	424	361
406	493	346	673	663	357	628	452	645	637	630
358	224	328	599	586	602	198	304	208	303	311
293	314	292	310	235	162	312	323	458	241	331
438	464	192	194	268	299	699	237	269	342	126
325	436	489	228	385	345	326	413	416	263	270
374	198	424	476	253	374	281	286	405	218	477
130	715	174	254	300	16	305	240	514	292	176
405	0	393	175	304	245	314	296	637	650	32
293	101	337	408	301	683	261	384	533	800	481
356	388	326	244	382	167	360	112	494	285	519
187	486	580	429	532	291	162	397	264	201	572
243	605	707	339	193	261	608	378	598	70	701
260	920	160	918	236	440	849	195	849	331	644
593	637	186	707	302	272	256	350	234	697	531
454	332	319	798	861	666	369	512	567	296	315
209	339	487	479	569	478	311	430	482	466	624
420	399	509	477	452	505	494	547	317	512	394
468	423	216	487	515	130	593	209	584	607	596
254	426	299	387	281	351	259	386	300	326	

1900.0_1135EC04	179	232	700	171	174	119	185	195	155	173	
	315	111	180	170	194	159	159	247	271	275	109
	150	235	125	164	302	153	200	118	167	203	62
	196	134	245	156	82	801	351	140	199	235	305
	254	187	164	187	135	263	237	174	241	195	183
	194	224	203	206	189	139	214	233	32	206	228
	259	107	242	247	212	267	208	251	319	254	247
	243	285	234	237	209	343	211	216	304	204	129
	160	115	149	3	126	294	242	211	243	184	127
	210	228	169	999	299	175	260	369	214	263	256
	112	111	70	101	232	233	177	283	230	269	316
	244	173	207	91	95	125	199	174	199	235	193
	213	199	279	207	202	223	935	246	450	103	267
	224	197	275	242	318	297	259	309	230	269	305
	277	159	186	209	193	271	210	152	205	225	213
	290	891	129	203	200	194	259	181	52	246	204
	149	3	161	0	869	169	279	251	211	874	163
	106	220	293	240	167	185	117	146	172	59	235
	168	0	258	278	212	170	0	0	120	0	176
	94	179	117	92	173	271	306	175	179	156	71
	126	75	200	59	86	192	243	68	96	109	14
	140	129	123	183	216	218	191	163	65	208	47
	187	125	151	179	77	154	167	218	180	44	299
	110	20	6	432	115	199	164	126	69	235	0
	148	244	23	0	139	2	188	52	205	192	225
	240	142	158	172	212	174	49	25	108	141	144
	0	202	140	50	202	92	86	226	65	66	203
	57	179	156	81	204	277	210	252	173	110	116
	91	1	49	305	86	117	108	32	154	267	300
	151	263	242	91	96	246	134	76	128	107	2
	11	131	310	62	279	66	261	80	19	215	199
	43	199	5	118	205	5	203	147	108	58	40
	256	61	309	356	198	160	162	174	139	161	

1906.6_1185EK19		291	332	259	321	289	293	289	229	697	238
	230	341	302	369	398	453	276	339	426	375	378
	434	230	497	261	260	450	343	300	649	390	650
	656	665	403	450	725	313	673	334	326	290	299
	245	302	539	315	206	342	334	197	276	292	462
	348	651	668	664	246	305	651	258	761	270	466
	264	813	510	467	267	347	281	494	377	354	284
	308	449	235	430	403	416	182	398	451	547	613
	618	598	637	257	628	144	905	615	928	680	576
	702	899	929	299	999	189	958	205	262	677	676
	262	808	795	765	346	421	226	510	272	493	602
	373	267	237	658	619	334	271	185	294	375	546
	320	373	242	271	311	261	297	351	274	260	257
	288	257	412	477	430	403	443	461	443	431	378
	411	517	363	679	665	380	629	460	658	640	642
	385	368	331	617	589	604	225	315	212	318	335
	294	323	310	323	361	226	344	371	466	350	335
	431	457	222	201	278	289	714	257	258	330	120
	310	436	530	264	402	334	324	411	449	263	294
	356	190	412	457	280	368	290	299	407	181	475
	129	730	175	261	306	15	247	233	501	282	177
	424	0	410	186	309	258	336	288	652	672	33
	314	122	356	416	284	694	240	403	558	820	495
	365	389	296	299	388	187	358	137	518	311	535
	170	505	604	441	534	289	185	400	270	215	598
	256	616	695	336	219	226	637	379	629	120	709
	268	874	141	866	257	415	829	214	833	346	654
	595	664	204	645	304	323	276	372	246	628	576
	457	335	333	787	827	672	390	540	586	342	367
	196	363	507	493	585	493	297	408	504	463	632
	415	350	552	489	483	506	513	557	321	554	401
	469	425	220	488	525	149	596	221	591	603	597
	263	414	313	417	306	363	272	391	303	341	

1908.3_1344EC04	197	230	160	262	233	133	216	265	218	217	
	280	181	150	186	194	164	190	196	223	247	143
	230	176	223	172	193	172	172	202	138	227	118
	142	127	152	185	162	232	196	145	176	220	269
	203	192	150	185	110	222	199	306	189	170	179
	351	188	154	133	201	203	166	252	152	225	167
	225	179	219	167	230	297	181	201	266	276	225
	280	245	271	188	225	285	352	140	228	241	112
	180	125	125	156	102	351	156	177	188	198	168
	206	143	160	175	189	999	202	252	197	205	214
	223	153	149	154	270	169	153	228	245	227	124
	175	154	239	198	165	184	239	206	313	235	208
	272	258	177	255	168	188	217	109	246	98	167
	254	164	260	273	256	255	254	266	222	263	291
	283	165	197	165	171	357	182	213	200	223	203
	248	222	164	196	191	179	276	161	105	204	217
	184	44	189	116	195	142	346	185	234	209	187
	197	169	269	156	135	216	189	287	209	196	245
	150	138	141	147	202	120	110	235	221	166	178
	150	160	176	203	168	231	208	137	131	168	157
	61	179	79	129	146	166	131	182	147	132	111
	195	168	189	194	193	119	334	157	118	127	12
	232	203	190	250	161	160	187	200	189	120	255
	119	138	150	197	132	224	258	171	200	198	135
	114	223	82	160	238	221	216	189	229	72	207
	171	163	157	203	211	141	97	129	82	272	141
	139	95	186	99	172	180	117	191	146	202	168
	145	164	185	142	176	315	197	225	176	121	193
	189	4	165	175	104	134	205	221	207	301	257
	198	218	199	172	123	181	123	139	146	196	193
	150	239	210	183	206	150	270	187	161	178	196
	151	230	78	99	215	136	94	229	154	120	194
	221	106	293	279	298	315	296	346	322	188	

1908.5_1185EK16	291	324	219	331	305	287	318	217	690	237	
	244	308	307	371	416	491	302	316	430	372	365
	405	237	491	261	266	460	345	291	662	364	664
	666	681	398	446	713	267	646	337	335	303	316
	270	301	554	324	237	350	331	215	279	283	444
	348	640	643	642	264	293	633	258	751	286	458
	284	796	511	453	275	338	286	485	374	345	272
	291	445	238	430	400	390	191	409	448	537	612
	621	593	620	261	627	141	940	606	934	655	567
	678	935	982	260	958	202	999	196	258	654	654
	281	783	773	746	322	431	194	523	249	503	574
	375	273	210	648	609	332	295	189	314	373	555
	304	376	235	244	275	254	256	327	269	280	238
	300	264	424	472	441	412	449	464	452	425	364
	410	500	359	671	657	386	623	438	647	636	630
	373	340	335	596	582	597	210	324	176	325	333
	314	333	314	332	335	205	346	337	444	325	353
	434	471	147	197	279	318	708	237	252	333	127
	324	448	522	254	391	344	320	414	414	269	299
	387	205	422	473	255	401	283	299	414	181	482
	170	721	177	256	298	140	280	235	508	303	211
	413	0	416	212	310	246	336	298	642	660	29
	311	121	343	411	264	678	261	391	555	806	484
	362	384	306	293	381	185	364	141	508	304	528
	171	488	610	423	528	289	183	406	274	204	583
	229	607	708	322	214	301	618	367	602	155	704
	266	881	176	885	254	434	814	224	815	329	642
	597	644	199	676	313	302	278	366	237	665	580
	454	239	324	766	826	682	347	526	582	317	351
	210	360	512	494	569	498	310	425	489	470	646
	411	360	518	499	479	511	507	531	309	532	404
	455	419	182	499	502	128	599	241	579	601	586
	261	406	317	409	302	373	290	392	318	327	

1914.2_2011EC35	291	323	236	308	308	329	299	218	241	236	
	197	298	753	287	181	226	286	180	163	353	327
	344	187	282	571	244	229	592	353	275	323	243
	279	262	198	210	258	285	313	395	317	329	197
	204	658	301	265	217	232	276	251	337	712	252
	289	249	237	243	247	274	241	303	231	269	207
	311	231	246	211	288	228	689	224	143	193	223
	209	191	462	217	225	249	209	258	173	223	203
	195	200	218	177	213	243	218	245	221	257	205
	259	221	199	369	205	252	196	999	497	253	251
	259	214	215	234	299	232	204	204	309	203	262
	207	175	146	238	259	230	327	899	295	352	241
	325	322	200	191	224	463	338	258	261	217	201
	330	481	219	214	230	245	204	213	237	294	227
	183	167	139	239	229	235	231	187	228	221	246
	191	330	232	217	233	219	231	160	222	158	207
	171	251	170	199	371	205	336	170	228	341	288
	292	207	230	818	334	299	255	235	210	312	147
	702	174	258	256	199	269	202	287	322	306	326
	257	570	321	369	299	181	373	391	215	107	263
	201	261	181	245	314	203	206	464	269	297	201
	210	309	221	159	271	292	299	276	229	240	25
	216	213	288	238	279	236	280	288	266	231	274
	273	142	322	292	253	603	204	444	178	264	242
	670	266	241	247	243	182	448	196	313	138	293
	169	217	272	246	616	109	211	242	215	235	282
	119	166	297	180	494	274	212	183	212	306	253
	217	249	679	242	155	275	401	272	740	262	210
	278	169	743	261	197	302	599	440	367	273	299
	213	254	328	235	238	188	235	232	203	211	265
	240	196	232	227	204	249	357	214	266	250	206
	213	247	149	233	233	263	268	255	242	230	212
	221	236	298	323	286	301	331	334	335	245	

1916.6_1164EK04	355	336	201	413	386	309	356	177	311	302	
	301	322	537	460	293	312	344	254	273	340	384
	389	228	355	499	309	287	464	400	314	459	284
	315	300	278	273	274	172	337	407	343	412	418
	549	548	377	308	195	433	505	282	326	633	308
	342	257	262	256	393	345	255	290	255	255	243
	292	267	247	243	309	249	556	228	263	205	525
	238	230	538	265	238	316	199	368	257	288	229
	241	252	253	343	256	197	292	315	281	273	248
	288	267	247	214	262	197	258	497	999	289	287
	206	252	254	253	342	244	274	293	266	290	228
	214	300	168	269	252	229	238	499	262	362	266
	274	337	271	231	412	566	190	375	335	289	198
	258	587	235	243	256	268	243	279	280	295	278
	212	209	264	270	268	226	271	242	252	264	257
	237	161	190	258	286	268	214	201	145	186	219
	210	211	189	154	196	213	294	231	229	181	387
	339	285	147	535	312	356	342	149	291	359	158
	540	251	285	255	253	335	313	322	399	253	357
	299	572	332	380	425	285	484	429	260	161	279
	361	318	251	394	425	282	548	543	346	364	190
	262	0	289	281	417	516	318	403	298	282	195
	336	108	394	281	302	310	382	381	304	285	294
	214	280	328	349	259	577	249	399	230	524	241
	463	318	258	185	283	243	493	273	286	278	425
	202	287	298	219	725	181	282	220	254	143	302
	280	236	138	260	948	232	249	219	256	360	318
	286	258	621	299	207	257	439	255	536	324	261
	258	58	553	305	275	412	451	465	433	278	299
	236	241	408	237	295	217	232	244	215	221	350
	263	206	281	389	411	288	357	278	228	275	298
	276	257	71	251	271	182	285	120	299	294	277
	268	220	298	302	282	298	241	309	302	272	

1920.6_2011EC41 298 301 199 326 321 315 307 248 603 231
275 391 293 367 416 426 253 442 436 385 424
462 257 510 287 263 507 350 341 502 429 478
496 487 507 550 787 245 715 398 387 302 386
250 345 637 362 219 373 368 285 296 313 617
328 641 652 688 298 379 648 320 768 281 468
306 786 472 474 252 461 273 489 376 379 325
369 536 255 474 371 496 225 411 515 619 716
693 632 682 252 696 160 643 669 658 885 602
887 639 642 263 677 205 654 253 289 999 994
355 648 662 730 348 585 257 521 359 523 640
619 295 293 690 703 593 293 232 375 463 660
354 382 240 355 328 195 278 342 304 296 274
336 210 436 457 452 438 441 496 447 466 496
492 596 505 672 683 516 649 582 712 655 689
494 312 315 664 605 627 223 451 228 447 464
429 440 434 457 304 320 421 483 580 340 348
475 405 173 209 288 307 641 238 125 390 165
267 430 564 271 493 353 419 466 474 377 282
309 193 275 359 321 407 360 334 423 261 569
213 776 231 294 360 96 260 253 590 363 230
468 2 471 278 388 340 369 351 638 701 136
268 177 415 505 341 716 186 464 598 812 622
329 322 198 306 431 244 386 189 628 331 711
179 538 662 421 633 276 263 402 293 211 655
317 731 636 313 195 273 737 479 679 145 628
370 574 160 602 270 493 705 204 718 369 788
684 774 222 649 387 331 240 367 294 640 717
447 163 359 646 612 635 361 518 628 354 309
247 352 585 553 687 571 301 455 627 453 560
515 445 686 553 562 493 521 699 398 525 491
622 477 199 524 666 162 602 262 649 659 687
391 532 377 432 406 406 314 453 355 342

1921.2_2011EC40 294	299	184	324	319	312	307	249	602	232	
273	385	289	369	410	425	254	445	436	373	406
464	260	508	294	269	501	347	344	495	429	472
487	480	516	549	787	226	711	397	362	302	389
252	344	642	365	215	377	364	299	303	300	620
326	643	654	690	300	371	649	320	770	279	456
307	788	458	461	251	456	271	476	375	379	329
367	538	248	480	390	507	253	417	500	620	719
694	632	686	255	699	176	642	669	658	885	601
888	639	640	256	676	214	654	251	287	994	999
360	630	646	731	346	586	252	524	368	525	644
620	279	296	697	710	601	301	230	375	461	668
360	388	235	356	331	214	267	347	293	292	270
342	217	437	459	453	440	442	498	449	459	495
493	598	506	672	683	508	648	585	698	653	678
498	288	312	666	606	629	221	434	224	435	449
425	461	424	454	290	320	434	483	581	317	349
471	395	173	207	291	307	641	241	125	383	167
265	426	568	237	511	345	420	458	472	376	271
306	217	286	351	322	404	354	329	434	227	564
183	775	232	271	329	97	262	247	568	369	227
468	2	470	279	380	333	367	346	638	702	159
275	176	411	507	341	718	213	463	595	812	620
328	322	196	323	435	255	387	203	632	334	715
177	540	653	420	631	272	255	420	286	200	658
302	731	643	310	198	266	740	481	682	165	627
369	557	175	586	268	493	704	180	718	367	785
685	776	228	647	384	328	247	364	293	637	725
446	163	356	628	594	634	360	512	624	351	312
248	344	585	546	689	571	302	456	628	454	560
515	444	694	543	543	496	513	677	398	524	488
619	480	189	524	665	173	602	266	649	660	688
394	526	377	429	414	410	322	467	375	345	

1924.7_1164EK03	227	232	0	248	235	254	208	220	365	128
215	269	213	294	229	262	157	226	228	289	244
321	223	411	234	272	268	301	235	347	308	319
348	327	310	378	361	0	334	235	232	279	182
265	253	337	235	213	320	276	252	270	237	366
303	303	302	292	250	202	282	316	342	257	313
303	347	339	321	243	305	238	330	258	290	268
259	243	217	269	516	415	283	197	270	332	291
285	314	289	195	294	230	313	328	295	319	310
316	283	267	112	262	223	281	259	206	355	360
999	293	309	328	301	304	236	270	635	283	302
289	279	394	341	339	307	544	255	316	292	276
870	302	196	446	226	165	100	281	292	298	146
564	174	273	315	333	302	267	372	402	442	316
264	271	298	327	325	335	311	295	322	379	334
366	0	223	308	343	349	292	313	229	423	340
340	245	355	337	54	298	319	404	303	0	249
262	275	177	213	203	208	392	225	126	245	164
221	258	305	218	278	247	228	316	375	292	163
275	160	241	323	277	289	199	191	302	250	372
151	343	160	183	247	115	257	225	316	240	218
282	301	309	165	239	232	302	209	309	323	240
260	183	224	319	256	331	157	278	348	357	350
192	301	190	227	224	217	318	108	273	285	323
168	317	287	217	326	249	167	266	212	0	320
219	319	309	235	210	167	290	235	297	225	304
285	235	230	312	209	286	312	233	335	305	316
293	339	203	298	235	262	151	231	279	281	295
264	75	242	316	272	320	148	269	305	261	233
308	231	257	280	347	271	303	249	249	253	271
233	240	274	346	273	333	378	306	133	286	242
295	261	175	304	337	135	309	169	329	331	310
227	236	299	288	324	340	284	362	310	218	

1927.7_1288EC32	257	232	118	315	311	243	325	234	598	211
256	300	259	294	367	387	273	284	327	337	343
390	216	429	238	263	387	272	308	514	357	510
501	505	384	483	705	165	619	282	320	255	310
278	295	571	305	179	307	269	199	264	254	457
301	617	650	654	253	277	615	292	750	259	418
301	787	473	424	260	290	236	461	359	329	263
339	412	228	497	341	428	188	418	451	550	667
653	545	634	278	615	111	812	561	841	635	523
635	813	823	111	808	153	783	214	252	648	630
293	999	979	852	307	399	211	513	292	520	644
412	307	260	754	705	377	258	221	274	361	554
316	304	273	284	243	158	101	275	280	224	220
274	153	435	471	456	438	453	471	440	471	431
474	551	359	658	673	382	640	516	684	654	673
403	155	316	636	571	590	219	392	275	427	394
385	399	422	434	151	268	311	408	506	142	315
328	407	101	200	233	325	621	216	167	291	105
283	387	483	253	321	329	354	356	378	305	213
247	148	223	319	256	349	212	229	327	217	474
205	658	87	216	281	41	272	206	511	289	203
400	0	430	256	273	259	303	284	570	649	31
242	167	316	367	279	655	202	384	540	794	490
320	343	327	230	434	188	331	64	551	269	577
147	495	643	423	534	255	174	319	177	216	564
293	626	682	286	179	297	689	346	677	120	672
412	798	125	817	207	374	966	201	943	337	589
572	706	191	663	224	238	191	318	224	662	578
397	195	298	857	893	745	405	525	601	271	232
165	323	535	550	574	513	294	437	487	457	529
409	395	480	540	506	516	422	548	270	455	436
513	399	195	502	591	189	532	126	568	562	565
293	413	264	316	276	308	251	334	235	270	

1931.1_1288EC35	258	234	64	316	312	244	325	237	603	211	
	254	300	260	300	366	387	274	286	310	342	344
	386	214	433	239	269	383	271	307	512	361	511
	498	503	391	489	713	78	622	284	334	258	313
	280	292	558	306	178	308	270	197	262	254	453
	303	631	667	670	254	286	632	297	767	260	420
	305	801	477	428	264	297	236	466	359	333	261
	344	413	227	490	340	432	189	414	455	561	682
	667	555	647	278	627	111	801	567	830	645	534
	645	802	812	70	795	149	773	215	254	662	646
	309	979	999	872	310	406	213	514	291	521	632
	413	306	263	764	709	370	259	221	278	367	563
	315	312	279	288	244	156	64	275	280	225	209
	274	152	439	478	462	440	457	477	444	462	435
	479	564	367	664	679	388	644	528	698	657	686
	415	96	306	653	585	603	221	398	279	440	402
	376	411	434	445	91	263	312	420	519	86	316
	329	410	106	200	234	325	626	219	166	292	102
	283	386	483	237	327	331	356	359	372	288	215
	247	148	223	322	256	353	218	223	339	217	480
	205	664	87	219	300	47	272	204	498	289	203
	404	0	434	256	274	257	305	285	572	660	13
	235	170	327	369	278	669	199	394	549	808	497
	300	343	326	221	451	188	331	68	563	267	573
	147	493	646	427	547	255	173	331	161	219	572
	293	631	682	285	180	309	706	350	695	104	670
	399	787	129	807	206	377	965	202	955	336	598
	577	706	193	663	227	234	182	308	225	661	586
	396	196	299	841	877	747	411	529	603	268	229
	166	316	541	548	580	521	302	439	495	461	530
	412	399	492	552	519	520	420	561	275	450	436
	528	403	195	514	604	181	537	129	585	575	584
	299	423	268	310	277	309	253	335	236	274	

1935.5_1288EC36	270	236	55	332	325	255	333	249	616	231
261	305	269	303	359	370	285	317	342	352	360
431	229	464	243	281	373	284	331	491	410	483
479	481	406	501	788	103	690	308	361	276	333
281	297	568	331	180	322	289	211	282	258	478
326	746	757	756	296	306	752	328	874	273	443
336	881	476	459	277	350	249	456	359	379	271
377	420	230	460	351	456	205	397	467	649	804
788	658	807	299	784	113	758	592	787	761	636
759	757	768	101	765	154	746	234	253	730	731
328	852	872	999	346	433	217	506	341	513	581
438	289	292	737	688	421	277	217	308	380	636
332	335	294	325	287	144	94	312	278	262	196
289	155	449	553	461	441	471	485	448	453	436
502	617	403	649	663	427	638	551	764	643	746
456	121	299	691	602	616	225	441	291	520	450
427	472	511	533	113	312	318	505	526	119	329
330	387	126	191	243	333	633	242	170	300	94
280	372	471	235	319	333	376	370	417	274	221
248	142	227	331	306	331	238	252	318	260	505
236	715	87	219	307	56	271	218	545	316	216
420	0	464	238	287	230	341	297	594	774	37
221	185	365	378	259	742	183	419	597	893	529
303	359	314	238	461	185	348	71	660	263	621
141	532	692	430	591	259	192	359	177	214	631
298	653	651	284	181	293	819	396	815	149	642
398	672	117	705	234	374	899	221	911	369	662
602	698	187	689	301	229	178	305	234	669	640
437	219	325	743	758	744	462	539	654	267	230
181	301	652	539	608	587	323	448	607	480	555
425	393	595	604	561	518	407	628	299	483	462
549	458	205	481	610	183	547	142	620	605	629
317	462	254	315	277	295	254	325	236	280	

1939.9_1185EK11	321	328	230	476	365	328	375	263	426	369
	202	377	352	431	260	290	341	260	314	363	528
	582	201	393	396	234	288	387	709	308	658	321
	320	318	298	337	377	263	349	373	498	366	181
	255	343	402	680	249	300	334	287	267	323	303
	770	337	353	353	335	350	350	215	363	256	285
	228	370	319	291	241	335	320	310	284	304	322
	255	280	305	217	338	275	239	226	276	328	344
	357	321	353	287	344	261	323	314	345	377	323
	372	326	319	232	346	270	322	299	342	348	346
	301	307	310	346	999	276	225	263	359	260	274
	244	214	202	313	319	242	321	278	325	329	270
	364	292	196	295	330	243	218	538	272	316	187
	329	277	266	257	280	268	230	271	259	335	229
	252	291	234	311	310	303	326	288	332	307	323
	301	215	235	289	326	322	206	242	73	249	253
	245	232	231	253	232	200	318	229	253	206	467
	400	346	312	332	345	375	443	289	321	408	103
	333	218	324	256	272	333	452	339	612	265	252
	301	243	333	388	595	298	304	435	345	146	342
	219	342	218	190	496	156	234	224	314	667	234
	227	356	252	203	371	319	737	299	302	367	83
	258	135	396	330	299	370	224	385	325	365	329
	211	250	271	269	290	320	269	178	397	305	294
	210	340	342	294	297	317	326	275	326	96	413
	202	290	343	255	275	204	346	282	336	269	278
	148	250	386	273	322	339	309	292	330	944	363
	273	345	306	330	333	286	270	272	334	345	271
	357	139	300	329	279	330	267	301	338	299	322
	255	258	361	332	308	293	227	253	320	190	287
	209	240	318	299	274	261	381	307	249	300	244
	260	261	95	276	301	158	337	223	305	323	263
	190	241	274	286	307	322	307	323	303	254	

1940.3_1288EC07	256	272	225	275	282	259	340	238	373	283	
	276	312	304	336	326	351	301	357	339	318	292
	367	289	354	275	292	354	298	300	413	317	391
	423	407	326	386	486	281	458	309	325	305	250
	225	310	429	229	174	252	250	200	303	275	492
	274	470	490	484	258	305	479	306	473	322	437
	315	476	475	427	322	265	244	443	272	308	242
	270	343	273	412	317	401	170	301	380	372	438
	443	363	467	322	453	140	434	464	424	518	382
	535	430	427	233	421	169	431	232	244	585	586
	304	399	406	433	276	999	242	415	295	415	571
	899	244	261	480	614	777	263	188	274	366	466
	344	317	224	305	344	237	221	347	229	172	209
	274	234	323	391	337	374	338	359	380	438	411
	327	418	304	502	500	390	460	443	468	477	469
	346	239	230	417	490	497	172	353	246	316	389
	358	315	315	328	197	298	326	386	428	251	273
	449	351	179	272	248	340	391	229	232	307	155
	296	354	450	253	400	361	299	395	372	343	245
	423	250	418	418	275	312	273	324	334	183	415
	214	507	145	243	312	32	230	269	407	239	151
	412	0	374	232	318	243	294	282	420	510	23
	289	128	339	345	295	437	233	287	381	473	423
	268	358	223	246	341	234	382	154	403	285	469
	196	396	376	267	451	254	216	314	205	218	446
	233	500	437	208	213	222	459	329	433	170	400
	410	407	145	415	225	423	431	229	442	283	510
	465	534	219	440	268	255	248	261	301	419	484
	353	75	304	413	360	360	267	342	380	246	276
	189	242	395	300	460	386	281	344	444	352	430
	340	312	387	332	318	343	373	463	243	397	333
	434	356	198	429	461	152	446	164	487	480	432
	213	374	298	351	284	333	201	350	302	249	

1940.4_1344EC27	295	328	123	281	292	291	318	92	284	187
186	291	222	283	157	232	269	170	149	316	207
289	256	278	254	207	299	297	232	309	310	289
320	295	291	252	256	107	244	334	340	303	168
227	218	281	183	306	319	303	223	305	240	227
235	210	223	220	221	303	211	213	260	259	255
227	236	230	251	223	199	182	227	207	180	314
218	212	242	211	208	243	207	219	165	244	182
171	228	181	281	185	166	240	271	216	256	218
255	188	193	177	226	153	194	204	274	257	252
236	211	213	217	225	242	999	182	230	182	197
215	318	189	190	208	219	237	199	122	286	172
289	345	224	215	368	318	173	246	338	291	185
230	364	238	204	232	228	251	297	261	234	178
224	180	154	252	254	190	247	200	240	236	223
234	91	227	242	278	284	226	158	37	184	141
147	35	140	150	129	154	262	195	221	85	268
255	121	117	172	266	318	274	108	223	346	86
151	172	251	77	184	221	212	241	311	209	470
232	228	376	364	307	233	285	319	267	127	222
389	193	197	325	331	202	195	257	254	185	277
142	0	165	175	278	272	204	201	263	225	161
309	0	326	209	243	245	244	291	220	267	279
209	207	102	298	166	321	211	134	213	297	146
216	187	248	149	235	169	234	144	167	218	292
103	207	362	250	249	2	212	200	201	111	321
11	208	228	211	267	185	201	54	210	220	284
232	194	287	277	226	254	236	268	220	290	147
176	5	153	245	251	247	169	234	266	241	282
211	264	257	183	296	191	250	152	169	215	259
215	215	200	272	260	244	327	248	75	216	175
226	255	218	216	257	220	242	66	256	267	231
164	184	265	268	272	233	251	246	231	267	

1946.4_1164EK02	302	299	159	257	270	306	270	270	683	221	
	297	351	330	398	536	483	241	363	503	308	327
	328	244	460	283	303	437	322	235	635	275	610
	652	648	427	515	556	219	550	320	290	245	289
	268	360	513	275	220	324	248	231	260	276	409
	262	420	429	432	248	277	421	327	502	304	438
	300	516	491	447	277	370	264	479	449	344	271
	321	403	292	390	367	453	208	386	382	439	419
	426	443	448	306	473	140	529	485	506	453	429
	453	500	501	283	510	228	523	204	293	521	524
	270	513	514	506	263	415	182	999	295	993	495
	441	186	152	496	494	367	276	219	310	400	417
	319	356	233	221	221	233	249	262	196	189	312
	288	212	326	359	329	305	322	337	323	421	324
	360	395	328	486	485	357	484	401	520	486	535
	342	296	315	463	439	455	247	310	258	350	308
	307	292	324	318	331	206	402	330	405	313	266
	430	388	181	177	279	270	661	288	167	391	209
	342	435	474	340	447	343	275	509	394	315	296
	327	231	281	386	192	446	346	295	443	167	496
	188	575	233	277	278	69	272	227	465	273	179
	472	0	414	281	338	210	253	270	505	449	80
	289	170	315	549	317	513	191	380	546	526	477
	398	340	298	303	400	265	363	203	370	295	440
	214	499	465	366	399	332	258	397	264	229	476
	379	456	473	345	238	332	430	289	411	168	465
	214	488	196	503	262	531	540	225	546	282	536
	433	543	270	429	414	307	230	365	274	428	462
	328	190	289	511	494	497	176	432	445	330	303
	187	359	387	433	411	409	265	286	320	319	495
	326	314	440	408	412	360	498	475	279	472	357
	390	351	167	469	451	175	396	245	426	432	445
	323	403	357	380	381	409	358	441	364	301	

1947.0_2011EC48	219	285	143	285	298	274	260	247	322	156	
270	298	263	268	251	248	230	228	169	307	264	
331	255	362	227	226	288	274	302	269	317	285	
261	265	270	338	376	169	354	246	289	332	278	
227	267	338	263	226	302	262	284	296	245	401	
318	319	301	304	331	211	298	289	345	252	306	
270	338	309	315	251	331	259	311	260	302	261	
259	274	270	258	632	364	268	233	282	326	301	
303	269	324	149	297	230	268	336	271	356	268	
358	255	241	230	272	245	249	309	266	359	368	
635	292	291	341	359	295	230	295	999	293	281	
299	309	556	356	346	308	369	286	342	292	269	
660	301	247	605	299	204	228	257	295	310	209	
395	199	257	302	274	278	254	320	322	382	305	
265	248	216	286	292	327	280	259	351	309	328	
312	199	184	282	280	288	324	414	197	517	434	
443	282	490	427	209	414	371	550	300	233	266	
274	239	245	191	285	260	324	240	124	344	137	
238	201	281	192	221	244	239	292	360	179	229	
228	193	250	260	233	254	263	281	215	143	316	
257	307	166	156	269	218	219	220	283	265	216	
211	262	234	223	291	211	304	247	258	297	34	
282	145	238	169	239	319	194	253	258	343	338	
223	183	162	256	201	244	243	165	267	268	249	
155	287	285	213	296	223	238	262	290	183	327	
214	291	280	215	241	233	313	273	282	228	325	
221	188	291	227	273	247	315	192	314	331	331	
308	324	285	323	235	261	197	247	232	284	256	
210	121	200	307	227	237	157	196	253	284	250	
261	246	252	289	309	252	258	187	244	242	213	
212	240	279	289	244	260	343	274	200	255	230	
241	289	201	227	282	142	247	245	269	251	275	
231	206	344	353	321	383	348	397	375	260		

1957.4_1164EK02	303	298	161	255	269	303	275	268	681	246
296	347	329	399	537	488	260	363	486	293	323
326	246	459	280	293	449	314	232	634	269	609
653	650	424	518	563	225	547	315	290	236	283
263	364	518	272	221	322	243	228	267	276	411
260	422	427	431	247	274	424	322	509	314	430
298	522	484	441	291	365	265	472	448	347	271
325	404	290	393	368	450	207	385	382	444	427
432	444	455	308	480	127	511	490	488	462	435
462	482	481	269	493	227	503	203	290	523	525
283	520	521	513	260	415	182	993	293	999	498
432	186	155	503	496	371	277	218	312	379	424
330	359	229	224	226	231	243	269	193	189	303
286	218	314	367	318	294	313	330	312	421	327
360	406	332	489	490	364	487	409	526	491	542
345	288	311	472	445	461	252	310	257	348	307
307	291	324	318	323	207	406	326	413	306	266
429	390	178	177	275	275	658	288	200	387	206
321	439	474	352	450	341	275	508	393	327	286
323	230	285	384	183	448	338	292	442	167	502
186	584	225	273	278	69	267	224	463	270	179
468	0	420	275	339	204	251	272	507	447	80
314	170	313	547	317	513	225	410	556	530	468
395	361	302	305	411	263	366	217	377	292	453
207	510	476	379	402	337	264	397	258	228	476
377	464	490	342	236	349	438	286	418	143	468
214	492	164	501	257	528	548	222	553	277	539
438	544	270	433	409	306	233	361	273	433	470
351	191	291	515	500	494	175	446	451	326	295
182	355	389	429	408	413	264	272	333	307	498
327	315	429	406	413	359	495	477	293	477	364
399	359	178	451	454	145	409	247	436	440	448
314	412	366	383	372	417	358	445	378	300	

1959.2_2011EC40	260	271	289	277	287	228	267	239	498	229	
	312	307	277	327	446	455	260	396	392	349	277
	382	261	428	223	226	402	314	262	410	334	433
	420	428	376	442	518	323	567	294	301	266	321
	315	331	613	274	187	376	316	159	244	252	588
	268	499	480	484	264	277	480	300	554	218	402
	268	556	409	400	231	320	273	388	382	301	276
	294	360	248	447	353	462	175	394	435	466	453
	478	420	460	269	490	125	579	500	583	568	426
	576	575	536	316	602	124	574	262	228	640	644
	302	644	632	581	274	571	197	495	281	498	999
	647	298	238	792	839	660	227	223	271	371	509
	291	307	301	281	285	166	313	279	314	226	201
	268	189	360	393	370	363	365	440	399	467	452
	375	457	349	562	564	399	511	465	521	531	539
	376	335	249	516	499	504	257	390	155	381	402
	406	356	379	379	344	304	320	378	483	317	287
	437	391	182	178	213	267	522	198	155	306	219
	258	375	633	249	421	328	286	382	375	412	169
	303	94	287	328	246	389	271	219	341	197	402
	185	562	60	247	272	16	300	230	575	261	155
	404	0	415	252	266	230	276	286	475	488	24
	177	141	293	334	215	510	131	317	427	611	374
	318	388	252	314	290	193	324	94	437	260	634
	97	423	548	357	436	273	169	331	194	153	472
	287	492	490	235	176	253	502	286	469	62	540
	18	604	162	632	208	443	641	218	655	284	529
	444	807	172	540	313	254	190	246	268	534	541
	312	136	342	697	619	554	230	429	439	267	259
	210	240	437	481	495	421	286	312	470	357	490
	331	365	466	430	434	393	375	498	273	510	422
	417	354	183	398	513	125	452	102	486	486	495
	275	400	283	365	255	279	170	294	220	268	

1961.3_1288EC07	237	257	239	233	247	261	277	231	409	213
	228	301	272	318	340	363	230	372	344	286	250
	348	250	351	227	261	339	307	257	414	316	400
	425	408	310	430	492	290	487	295	267	275	258
	195	293	492	211	182	267	252	208	245	232	576
	239	449	539	522	230	271	521	287	466	281	404
	299	435	417	406	278	273	226	402	268	288	228
	288	323	245	377	300	392	160	306	397	394	451
	454	396	413	232	457	185	413	447	402	499	371
	516	389	373	244	373	175	375	207	214	619	620
	289	412	413	438	244	899	215	441	299	432	647
	999	241	233	566	709	873	242	194	208	355	460
	299	326	179	279	288	218	248	306	204	172	194
	254	235	297	360	296	343	311	348	372	433	385
	307	406	312	469	460	379	426	436	466	447	466
	317	274	250	397	468	461	174	282	220	285	329
	292	291	292	296	221	284	332	341	426	244	245
	445	366	167	239	249	277	428	234	183	282	144
	284	369	518	248	427	315	246	381	376	425	227
	384	235	360	397	269	292	254	263	348	185	450
	158	513	151	222	264	28	219	214	471	220	121
	356	0	333	212	274	231	248	253	430	480	16
	288	137	306	358	232	429	252	302	421	493	407
	306	306	203	236	328	202	365	201	404	296	579
	176	390	404	272	427	250	206	283	216	207	448
	234	481	439	230	189	256	483	325	466	159	407
	398	438	115	460	221	437	420	230	455	274	502
	450	606	208	431	267	243	253	262	288	409	470
	341	72	295	432	413	367	259	362	388	233	303
	192	250	371	311	438	356	261	301	418	297	442
	344	341	410	337	337	347	385	452	267	413	353
	420	335	204	412	452	126	431	131	464	450	412
	210	364	307	366	303	344	209	362	313	259	

1975.9_1344EC27	237	283	141	290	280	228	225	170	243	208
	180	263	203	296	208	260	183	251	233	246	198
	327	269	299	252	242	294	235	251	265	358	262
	286	267	239	237	232	136	245	293	262	347	236
	255	313	249	196	220	353	275	235	255	266	247
	217	188	224	210	328	290	212	249	260	195	263
	225	262	293	240	200	195	226	256	186	234	310
	217	194	261	235	273	277	198	185	212	304	197
	202	269	204	317	246	181	345	260	344	208	270
	208	339	331	173	267	154	273	175	300	295	279
	279	307	306	289	214	244	318	186	309	186	298
	241	999	199	301	277	214	251	136	137	298	218
	277	324	217	200	342	364	136	327	769	737	196
	273	335	240	230	233	275	232	225	285	272	210
	214	269	194	303	288	168	276	263	271	276	269
	208	138	242	274	301	286	219	204	69	193	195
	160	205	141	152	183	173	297	190	261	140	284
	266	204	142	205	224	225	259	226	193	283	116
	183	199	241	216	273	271	197	277	335	248	291
	269	210	354	330	320	254	286	288	244	64	237
	300	244	189	280	283	64	247	238	290	188	185
	198	0	254	235	294	290	228	283	305	234	187
	344	146	309	241	268	252	270	314	265	269	244
	260	263	190	284	237	271	258	184	225	307	195
	169	255	285	218	244	253	243	233	235	211	362
	228	231	266	264	282	88	221	160	225	282	275
	15	315	216	328	326	231	296	186	326	237	272
	223	292	270	341	255	266	294	287	237	353	274
	270	10	180	346	335	324	173	291	319	253	261
	711	284	359	283	291	225	276	260	187	219	283
	255	224	250	299	301	288	329	268	117	310	224
	266	216	254	286	275	179	312	121	332	307	277
	192	240	300	308	327	333	335	299	277	255	

1985.5_1164EK03	205	211	164	169	158	210	159	250	333	119	
	198	281	146	251	183	208	177	208	122	195	172
	375	253	372	225	184	219	203	201	249	280	255
	232	230	175	237	336	218	328	215	176	288	200
	179	180	234	166	200	171	263	224	196	157	309
	258	309	303	316	231	125	296	198	303	234	313
	182	281	346	318	241	218	189	342	177	262	159
	198	177	174	191	398	214	222	217	173	278	275
	281	251	293	180	235	175	244	279	251	284	261
	282	227	196	207	237	239	210	146	168	293	296
	394	260	263	292	202	261	189	152	556	155	238
	233	199	999	240	244	192	332	153	268	234	255
	478	241	177	963	251	192	226	290	177	197	222
	293	166	221	225	235	243	212	228	210	277	212
	206	209	170	287	278	202	248	303	313	223	277
	229	255	272	244	263	269	255	368	295	432	373
	490	279	413	458	208	475	296	488	230	235	177
	183	148	208	186	227	159	322	273	117	289	202
	114	252	229	245	220	206	193	287	410	191	282
	164	186	209	275	281	153	179	216	182	165	269
	117	308	205	165	193	178	163	173	210	193	185
	204	158	228	158	223	188	257	205	289	284	27
	294	219	169	141	226	279	204	266	208	309	203
	234	125	116	256	197	199	225	178	275	162	243
	149	240	226	193	334	157	191	261	248	118	354
	170	303	279	295	206	0	315	264	302	269	307
	319	237	280	236	163	136	275	103	284	252	271
	325	288	172	257	178	288	182	302	139	247	266
	235	101	172	273	236	214	191	201	224	283	282
	232	305	187	227	305	183	142	159	218	177	194
	121	185	269	213	201	209	360	308	184	254	158
	289	213	190	214	333	176	267	216	244	230	294
	151	145	289	334	331	332	328	342	307	274	

1991.6_2011EC38	276	249	118	345	344	269	318	212	575	292	
	281	350	285	357	419	393	300	367	452	325	278
	454	255	477	269	223	398	306	295	518	385	528
	496	494	415	495	634	176	590	334	306	273	353
	279	312	726	288	213	335	297	197	264	271	685
	314	580	572	576	283	288	567	337	688	250	447
	318	706	468	457	264	324	292	449	370	339	265
	327	362	249	472	390	461	173	413	478	575	617
	640	545	608	237	645	139	665	541	673	702	534
	703	659	637	91	658	198	648	238	269	690	697
	341	754	764	737	313	480	190	496	356	503	792
	566	301	240	999	900	607	257	255	300	401	591
	311	350	297	301	284	175	95	326	271	279	228
	296	205	334	436	370	337	349	405	368	450	433
	421	515	450	572	584	423	541	494	607	557	600
	453	107	313	575	517	526	232	443	259	459	450
	444	387	441	461	109	304	324	470	506	100	338
	427	401	130	259	261	318	602	207	212	351	138
	270	362	643	205	439	326	311	449	458	482	255
	290	187	249	321	293	381	286	310	367	178	481
	201	676	191	269	256	62	279	248	673	305	190
	454	0	461	275	296	235	344	303	529	590	41
	224	147	319	465	218	655	212	384	522	765	447
	317	362	255	258	384	198	341	165	526	279	790
	165	475	618	384	512	273	185	418	224	261	547
	260	601	583	294	191	250	664	271	630	116	668
	360	678	137	678	236	407	765	179	788	349	631
	536	903	199	599	314	238	200	320	245	604	617
	372	154	384	705	696	658	348	519	574	272	255
	214	318	511	536	538	537	325	378	540	391	593
	390	379	525	508	484	439	424	578	339	556	407
	467	380	173	394	543	196	482	176	540	552	550
	292	365	287	355	323	337	165	367	294	286	

1997.0_1288EC09 260 251 120 334 340 236 322 214 540 254
282 324 278 329 362 380 268 331 430 352 307
429 241 442 260 201 392 324 304 480 389 473
469 470 384 449 614 165 574 312 327 293 353
288 293 672 288 191 337 295 174 255 276 634
293 588 567 573 294 284 563 333 652 244 439
321 677 463 442 259 308 303 433 333 333 257
303 410 246 461 366 470 177 374 465 541 589
608 500 582 276 612 129 634 546 636 669 512
670 622 605 95 619 165 609 259 252 703 710
339 705 709 688 319 614 208 494 346 496 839
709 277 244 900 999 727 260 263 297 383 553
325 344 282 297 316 144 98 329 261 258 278
297 202 349 419 366 361 361 433 396 456 468
377 488 410 591 602 424 549 484 603 567 608
430 126 301 577 529 542 261 438 256 429 447
410 381 418 443 110 289 315 447 508 128 348
399 372 127 249 242 322 570 202 144 327 123
289 379 593 172 402 328 334 427 422 442 230
277 151 248 342 312 365 267 259 350 160 432
241 636 163 265 281 61 298 247 624 293 186
420 0 444 254 310 249 321 263 531 590 41
214 105 321 417 207 605 166 352 510 723 439
311 391 258 255 353 184 334 149 491 270 727
165 423 552 351 531 260 185 373 211 161 518
266 612 547 266 188 230 626 328 593 138 583
392 608 114 622 211 435 718 178 741 344 610
561 930 186 604 304 234 155 302 298 599 574
371 125 381 672 658 614 324 461 524 244 247
188 299 502 504 561 489 326 393 521 385 517
398 365 487 491 493 433 413 544 299 518 388
452 380 158 427 541 193 497 158 539 560 572
278 371 282 326 299 309 207 332 252 277

2014.0_1288EC06	256	258	57	266	296	239	284	231	391	209
289	323	293	318	401	383	256	379	376	338	252
329	255	357	241	236	335	309	250	360	292	353
364	354	327	459	470	3	444	259	244	290	321
257	294	534	229	161	305	276	212	283	262	654
238	443	431	435	239	266	429	289	434	244	335
279	418	345	341	260	307	285	336	311	304	218
287	363	222	364	323	401	160	340	428	382	392
426	353	404	246	417	159	340	424	330	538	358
541	325	323	125	334	184	332	230	229	593	601
307	377	370	421	242	777	219	367	308	371	660
873	214	192	607	727	999	229	218	231	321	458
296	284	227	266	267	121	123	274	230	212	171
266	161	258	336	291	311	285	350	351	436	430
307	367	299	414	414	404	380	435	432	419	422
329	87	264	398	408	403	207	375	263	382	394
355	314	350	364	101	303	286	393	416	91	290
433	338	99	252	229	284	407	225	86	326	143
295	368	549	233	406	327	277	397	353	475	208
271	85	258	310	241	338	257	225	332	182	437
235	493	113	245	237	4	295	253	503	236	148
393	0	354	266	252	199	258	236	404	441	0
242	130	273	355	234	449	159	299	396	459	353
286	371	242	240	331	203	348	84	358	257	576
126	336	405	314	402	269	138	303	182	138	433
276	490	341	241	159	304	463	291	405	171	372
340	323	92	348	175	443	413	264	406	283	486
445	670	169	385	267	206	105	245	302	372	482
310	95	287	389	352	345	224	389	368	226	207
172	227	360	351	433	335	246	257	419	284	348
356	299	390	339	317	324	382	436	258	401	379
421	317	149	334	471	213	388	166	410	398	401
214	346	256	276	255	291	200	313	244	218	

2066.6_1164EK03	220	263	40	230	239	202	250	243	325	184	
	257	246	263	196	170	193	199	180	104	326	263
	329	214	293	202	144	229	267	282	314	321	220
	301	269	219	240	292	113	280	244	251	302	205
	156	211	260	224	236	303	282	289	262	247	277
	347	290	273	271	271	190	272	364	282	300	256
	323	302	291	258	256	332	244	274	206	264	217
	266	218	262	239	329	405	255	212	273	334	248
	237	227	269	137	223	255	272	286	274	300	226
	287	269	266	199	271	239	295	327	238	293	301
	544	258	259	277	321	263	237	276	369	277	227
	242	251	332	257	260	229	999	296	304	303	244
	613	314	272	344	237	197	189	244	268	212	209
	969	198	304	339	315	331	313	387	417	406	352
	271	241	230	252	266	319	263	258	284	302	262
	401	139	222	224	268	267	325	258	117	316	288
	223	57	286	257	162	231	347	355	255	137	238
	165	233	267	200	230	250	315	250	79	254	99
	214	111	227	49	157	204	143	236	305	147	176
	175	149	187	257	284	194	222	266	104	0	216
	203	262	134	82	207	115	136	186	219	202	243
	129	224	199	129	274	194	336	138	169	311	1
	228	191	244	152	203	262	153	230	207	271	315
	213	79	218	156	157	239	221	102	173	172	184
	182	230	213	172	226	203	256	251	235	0	240
	185	172	302	229	212	94	242	224	232	216	276
	220	191	213	246	220	239	254	217	276	308	293
	241	249	244	290	176	282	92	223	250	259	204
	237	3	183	287	234	198	201	133	268	294	291
	255	232	215	223	240	255	287	219	199	244	109
	122	270	231	320	244	340	356	242	67	135	209
	190	328	140	200	293	181	206	205	251	240	211
	240	176	310	287	323	311	288	341	340	241	

2075.8_2011EC34	267	295	162	283	300	327	308	245	233	247
	186	284	737	270	226	259	272	210	152	338	293
	287	167	261	559	234	227	561	350	290	327	248
	304	271	222	238	243	166	211	366	331	338	147
	177	677	298	253	187	257	240	233	353	766	256
	288	267	226	252	253	229	246	336	220	280	206
	325	205	237	212	311	257	775	232	181	288	240
	270	223	493	217	225	256	170	267	221	254	218
	199	219	213	247	181	153	203	258	203	251	211
	250	203	192	174	185	206	189	899	499	232	230
	255	221	221	217	278	188	199	219	286	218	223
	194	136	153	255	263	218	296	999	261	318	277
	279	283	246	177	257	449	181	290	206	184	152
	271	450	223	226	234	266	220	214	235	280	256
	190	202	219	223	211	234	204	202	230	228	226
	228	182	221	243	224	207	154	198	86	203	274
	218	158	199	227	161	208	322	202	266	174	288
	267	196	139	822	315	308	272	287	241	314	194
	699	204	279	238	247	288	146	304	290	288	315
	246	562	336	365	282	158	380	396	232	141	269
	179	258	250	213	332	236	175	479	287	266	186
	187	29	263	178	269	253	297	258	235	245	0
	213	114	225	286	275	200	252	307	279	211	272
	266	197	322	244	239	652	304	478	211	258	273
	665	218	229	224	247	293	453	218	234	88	286
	168	248	258	237	648	191	216	267	192	206	275
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	222	231	775	217	247	220	369	239	755	220	241
	292	136	749	243	191	314	587	437	358	217	249
	162	236	315	257	269	199	119	225	214	200	278
	242	208	212	241	164	245	319	237	152	182	231
	250	248	97	210	264	237	278	233	237	218	232
	209	238	252	264	238	274	295	300	310	215	

2086.8_1344EC29	363	277	188	251	247	329	231	251	394	155
196	274	320	334	312	326	179	259	289	352	324
275	215	350	353	211	341	342	314	367	356	364
361	364	314	402	385	172	379	335	261	248	137
193	293	368	256	205	359	237	358	233	274	334
350	306	332	315	207	290	317	330	326	314	256
316	351	287	252	302	284	264	275	288	333	240
299	321	259	248	387	330	325	194	295	331	259
284	280	287	244	273	275	311	354	311	371	285
382	304	284	199	294	313	314	295	262	375	375
316	274	278	308	325	274	122	310	342	312	271
208	137	268	300	297	231	304	261	999	344	315
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310	318	263	315	297	304	240	328	308	378	269
274	263	245	313	311	253	310	276	307	320	302
185	178	191	292	316	300	254	260	164	238	266
287	168	247	226	160	215	368	249	265	193	273
414	326	487	265	334	231	419	256	186	290	128
298	345	368	249	288	307	280	409	360	220	315
407	247	330	382	313	299	280	266	323	123	385
86	431	165	263	334	102	170	299	300	282	190
283	480	257	196	274	234	341	223	361	321	26
304	237	309	325	170	375	263	336	398	377	384
217	307	179	229	296	296	328	191	290	264	332
228	351	255	280	321	318	251	276	337	112	406
182	324	305	256	279	171	333	246	317	275	343
136	281	412	339	283	365	293	200	319	362	394
321	342	250	360	255	306	287	262	285	357	292
297	46	322	308	277	339	323	353	397	310	282
174	246	344	329	307	313	252	283	283	276	376
236	249	313	270	281	291	399	331	203	395	236
291	244	112	307	314	167	326	260	323	342	299
248	240	334	311	304	374	359	376	347	233	

2089.0_1288EC05	325	363	195	370	357	356	357	262	341	277
340	303	348	423	313	371	364	327	281	459	393
405	297	365	384	277	402	381	370	377	335	319
389	365	428	385	388	227	421	450	413	346	358
260	407	342	312	178	391	342	286	351	392	404
307	397	406	406	338	432	403	364	372	338	397
332	376	395	406	332	401	375	396	312	320	336
338	314	408	370	285	398	248	396	318	387	378
379	372	390	380	388	240	396	387	393	452	391
460	388	367	235	375	235	373	352	362	463	461
292	361	367	380	329	366	286	400	292	379	371
355	298	234	401	383	321	303	318	344	999	375
327	355	330	269	349	400	221	320	349	322	249
319	376	361	391	383	384	360	410	381	444	381
326	387	377	424	419	413	413	397	417	434	396
445	221	320	407	449	439	266	304	201	318	302
283	237	294	274	271	281	389	348	383	217	335
558	314	128	316	341	357	359	255	220	373	182
314	323	409	253	354	403	260	385	427	260	336
378	308	348	358	284	296	415	418	331	187	406
314	439	309	263	392	194	260	277	342	332	203
315	0	401	300	446	337	306	321	372	419	123
264	144	458	378	349	395	284	439	313	395	444
309	204	301	347	285	384	296	294	346	354	348
263	355	408	232	350	323	387	316	370	229	472
257	376	432	341	349	189	397	284	401	226	463
297	367	152	342	359	348	378	221	372	336	478
365	372	346	421	360	360	311	393	419	398	402
344	223	350	409	379	439	356	408	461	364	379
272	379	455	383	337	348	289	324	331	366	355
317	305	471	408	407	384	401	454	278	379	368
413	387	253	375	432	217	386	244	446	398	352
375	341	388	441	384	396	285	422	403	334	

2091.4_1288EC40	254	242	165	310	296	231	289	263	445	215
227	256	252	282	382	389	258	338	405	330	316
348	224	366	219	203	349	262	264	342	317	347
353	352	404	487	628	231	586	317	271	246	319
240	303	436	259	161	312	264	253	262	280	471
285	582	575	579	228	276	574	317	620	251	369
302	587	386	379	235	371	237	370	246	344	245
346	387	217	452	351	453	234	350	488	517	573
572	525	575	218	573	191	529	507	556	633	516
630	549	537	193	546	208	555	241	266	660	668
276	554	563	636	270	466	172	417	269	424	509
460	218	255	591	553	458	244	277	315	375	999
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269	168	418	461	420	422	441	458	432	475	454
600	496	417	582	573	394	512	534	566	519	546
380	194	301	501	471	490	237	415	293	440	435
393	407	425	454	204	348	357	464	479	220	324
323	329	96	240	221	289	467	252	113	268	120
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157	547	213	268	231	83	237	234	430	273	131
512	4	428	247	267	243	309	295	451	601	95
219	188	315	368	252	588	169	373	414	615	466
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144	429	530	344	565	258	188	406	228	231	561
283	610	458	287	162	221	598	394	567	221	453
394	478	108	517	246	403	602	211	617	306	540
581	596	202	537	338	229	162	323	203	504	952
373	128	303	537	508	476	248	457	484	241	216
214	314	472	426	522	501	322	422	515	430	384
440	506	575	474	455	452	385	558	315	434	427
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294	415	278	299	303	284	242	330	276	290	

2101.9_1164EK03 205 304 147 283 301 260 284 238 357 166
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2127.8_2011EC19	317	404	171	296	317	371	305	194	329	186	
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	381	354	263	289	352	189	319	338	381	351	254
	206	318	380	298	287	340	308	335	338	306	325
	311	361	353	351	341	347	355	304	331	283	327
	274	341	375	333	273	324	304	357	257	254	309
	247	275	318	270	348	377	337	291	293	360	321
	345	324	334	244	356	226	369	362	373	378	325
	388	366	375	199	373	258	376	322	337	382	388
	302	304	312	335	292	317	345	356	301	359	307
	326	324	241	350	344	284	314	283	383	355	302
	335	999	302	304	415	313	185	316	335	330	200
	346	342	296	320	299	306	289	337	322	392	306
	274	306	229	375	368	339	350	305	338	361	361
	315	173	238	318	344	348	257	251	108	246	276
	156	118	257	227	180	183	321	276	304	177	285
	338	269	227	234	361	305	321	170	178	356	154
	256	219	327	194	206	283	178	307	375	299	343
	331	221	389	351	278	247	293	365	212	33	304
	213	327	123	170	380	112	187	256	301	291	287
	257	125	261	199	319	237	277	286	247	365	135
	319	135	378	165	259	331	276	277	243	340	357
	341	204	207	312	231	330	221	189	266	291	287
	256	324	328	171	296	189	301	267	291	152	377
	239	212	336	248	301	140	318	259	293	176	363
	214	285	163	275	326	255	315	196	321	274	376
	269	342	318	385	206	322	279	282	292	353	268
	259	120	228	337	298	394	252	273	400	333	318
	300	271	353	236	267	285	275	237	241	256	303
	187	261	268	332	334	309	325	292	147	269	294
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	271	228	328	361	338	356	277	327	314	280	

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	294	294	263	276	295	297	364	329	300	290	241
	252	321	264	268	200	276	280	269	256	262	260
	248	199	224	209	268	302	209	242	274	221	192
	227	279	255	195	256	256	229	209	240	240	298
	267	245	276	254	228	340	297	218	274	240	204
	213	246	246	228	237	328	269	241	273	253	242
	254	251	227	279	242	177	235	200	271	240	235
	196	273	279	294	196	224	224	233	247	229	301
	179	217	177	297	282	227	272	246	230	330	269
	236	302	999	171	198	258	267	279	271	224	217
	300	271	203	245	220	243	172	246	241	351	269
	265	201	264	251	254	211	235	238	239	262	253
	421	290	234	243	229	217	227	220	243	256	215
	138	282	194	262	338	188	288	137	263	299	255
	373	336	200	316	256	312	305	242	282	304	264
	233	249	263	298	311	289	209	303	295	259	338
	298	241	295	316	279	271	334	293	282	94	261
	208	295	263	223	287	60	250	241	306	254	182
	258	146	297	267	285	293	289	255	241	219	23
	244	252	327	284	254	283	270	286	263	273	258
	243	284	221	309	281	238	246	205	241	322	257
	123	309	318	162	259	241	255	257	294	283	300
	256	262	197	257	259	184	232	207	278	296	256
	204	224	199	247	274	271	286	165	283	280	260
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	149	269	287	241	283	225	298	219	269	173	332
	251	249	264	234	268	256	330	277	210	295	256
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346 339 201 316 220 288 206 269 191 323 299
268 172 204 305 260 280 188 259 284 301 287
251 272 223 231 342 234 256 207 265 205 264
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316 292 200 280 347 156 297 241 287 281 329
224 237 324 337 340 366 335 376 335 278

2174.2_2011EC19	330	289	184	338	347	324	325	157	292	237
227	368	262	380	301	333	327	339	272	403	276
448	165	370	338	246	340	329	368	316	554	307
322	303	278	300	298	199	346	341	371	607	218
243	326	353	289	209	321	474	206	327	302	330
329	285	314	296	555	328	303	241	294	215	353
233	296	358	352	240	267	319	316	247	248	426
228	252	332	250	300	311	217	257	278	296	307
289	267	312	392	313	189	303	275	322	328	255
324	282	266	202	311	168	275	224	412	328	331
226	243	244	287	330	344	368	221	299	226	285
288	342	251	284	316	267	237	257	237	349	261
305	415	198	308	999	353	192	612	359	374	167
268	361	268	272	284	278	255	280	294	313	263
278	279	241	310	296	246	299	274	319	316	310
267	187	223	235	313	304	230	206	151	236	253
261	136	212	240	160	263	341	257	258	164	339
373	325	125	257	334	325	326	172	223	429	27
245	280	283	254	328	316	204	239	490	206	316
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655	250	260	324	342	413	230	249	320	297	200
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375	97	401	265	365	298	224	427	238	337	334
249	234	182	291	195	306	216	185	265	394	228
181	272	408	107	273	239	300	260	255	207	392
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183	253	189	292	406	282	271	109	329	298	360
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316	30	222	328	261	330	207	324	344	299	293
365	227	329	297	261	247	236	232	187	209	296
283	236	253	333	306	304	397	324	160	243	257
278	247	160	287	296	188	286	211	320	313	297
218	278	338	342	334	348	275	333	324	240	

2197.4_1344EC14	324	367	210	312	326	335	366	143	181	281
	329	280	468	337	172	218	328	197	123	406	301
	359	248	195	465	275	259	417	329	318	349	202
	302	262	149	152	166	218	223	451	352	346	269
	271	473	181	256	197	369	363	249	377	580	165
	265	266	272	278	340	391	277	315	151	267	267
	304	154	282	260	288	264	552	266	247	149	334
	157	151	601	179	199	273	224	307	197	321	235
	249	298	249	319	257	261	248	170	254	176	296
	186	255	253	223	261	188	254	463	566	195	214
	165	158	156	144	243	237	318	233	204	231	166
	218	364	192	175	144	121	197	449	269	400	130
	213	313	258	195	353	999	212	310	427	390	222
	203	660	248	249	269	283	246	289	311	272	217
	135	143	249	211	215	211	210	137	217	246	220
	231	182	241	160	225	214	197	132	76	160	177
	87	133	159	160	187	115	301	182	191	177	275
	274	216	164	495	324	366	193	165	222	268	235
	434	187	191	166	178	327	89	242	323	113	355
	286	474	387	319	337	188	426	463	120	43	171
	309	181	240	268	327	225	267	478	182	271	193
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	198	116	212	332	181	618	145	423	105	326	147
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	89	118	207	280	294	291	301	160	70	143	212
	124	244	86	206	174	190	165	98	199	147	117
	183	105	270	310	253	248	148	275	253	183	

2200.0_1135EC03	194	246	714	175	172	118	170	146	156	154	
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	186	132	232	156	76	814	313	130	194	230	279
	224	184	137	183	173	218	209	175	188	180	175
	186	203	179	183	198	137	186	166	32	165	198
	191	122	240	215	182	238	197	229	344	208	246
	204	272	223	218	211	307	198	191	310	191	118
	151	107	133	5	118	299	209	223	218	202	115
	227	205	161	935	297	217	256	338	190	278	267
	100	101	64	94	218	221	173	249	228	243	313
	248	136	226	95	98	123	189	181	198	221	204
	215	185	267	180	192	212	999	241	448	118	263
	209	188	254	224	272	279	224	266	205	251	277
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	108	193	306	248	164	170	119	87	166	59	247
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	90	178	115	110	178	264	297	186	184	143	67
	136	78	240	64	87	219	210	60	96	108	126
	118	130	119	221	225	209	196	139	58	183	46
	221	136	152	144	83	135	178	189	152	46	259
	108	21	6	411	177	216	87	138	82	237	63
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2206.1_1164EK04 328 251 139 433 352 290 394 174 382 357
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308 120 279 280 106 281 285 318 240 153 419
334 311 97 266 303 394 394 180 288 343 19
298 322 309 248 330 342 370 294 570 164 189
386 86 402 395 659 332 420 334 279 206 314
518 273 316 224 407 426 257 185 294 529 176
187 0 216 246 371 384 564 303 271 376 2
220 94 407 243 340 322 106 406 310 348 326
162 265 222 211 215 304 263 171 357 355 261
200 307 369 249 230 236 285 249 169 12 404
119 247 288 179 322 238 324 234 354 84 243
3 288 165 317 363 311 295 300 309 569 358
244 345 255 315 219 171 205 173 241 320 277
238 143 202 279 276 311 205 273 322 195 199
324 166 293 335 232 276 202 223 275 231 212
227 275 313 305 262 306 305 277 149 275 217
252 285 45 283 249 207 315 105 315 301 263
191 196 230 246 159 249 177 235 203 222

DEMANDE OU BREVET VOLUMINEUX

LA PRÉSENTE PARTIE DE CETTE DEMANDE OU CE BREVET COMPREND PLUS D'UN TOME.

CECI EST LE TOME 1 DE 4
CONTENANT LES PAGES 1 À 361

NOTE : Pour les tomes additionels, veuillez contacter le Bureau canadien des brevets

JUMBO APPLICATIONS/PATENTS

THIS SECTION OF THE APPLICATION/PATENT CONTAINS MORE THAN ONE VOLUME

THIS IS VOLUME 1 OF 4
CONTAINING PAGES 1 TO 361

NOTE: For additional volumes, please contact the Canadian Patent Office

NOM DU FICHIER / FILE NAME :

NOTE POUR LE TOME / VOLUME NOTE:

CLAIMS

1. A method for analysing the metabolites of a biological sample which comprises quantitatively determining one or more metabolites in said sample in a way that said quantitative determination resolves isotopic mass differences within one metabolite,
said method being characterized in that the sample comprises or is derived from a cell which has been maintained under conditions allowing the uptake of an isotopically labeled metabolizable compound so that the metabolites in said cell are saturated with the isotope with which said metabolizable compound is labeled.

2. The method of claim 1, further comprising, prior to quantitative determining the metabolites, combining the biological sample (i.e. the first biological sample) with a second biological sample in which the metabolites are not isotopically labeled or are isotopically labeled differently from the first biological sample; and determining in said biological samples the relative quantity of metabolites which differ by their isotopical label.

3. The method of claim 2, wherein the first and the second biological sample correspond to different phenotypic and/or genotypic states of the cells comprised in the samples or from which the samples are derived.

4. The method of claim 3, wherein the different phenotypic and/or genotypic states are different developmental stages, environments, nutritional supplies, taxonomic units, wild-type and mutant or transgenic genomes, infected and uninfected states, diseased and healthy states or different stages of a pathogenicity.

5. The method of any one of claims 1 to 4, wherein at least 50 metabolites are quantitatively determined.

6. The method of any one of claims 1 to 5, wherein the metabolites comprise sugars, sugar alcohols, organic acids, amino acids, fatty acids, vitamins, sterols, phosphates, polyamines, polyols, nucleosides, adenine, ethanolamine, nicotinic acid, uracil and/or urea.

7. The method of any one of claim 1 to 6, wherein the isotope is ^{13}C, ^{15}N, ^{18}O or ^{2}H.

8. The method of claim 7, wherein the isotopically labeled metabolizable compound is U-^{13}C-glucose, $^{2}H_2O$, $H_2{}^{18}O$, U-^{13}C acidic acid, ^{13}C carbonate or ^{13}C carbonic acid.

9. The method of any one of claims 1 to 8, wherein the biological sample comprises yeast cells or plant cells.

10. The method of any one of claims 1 to 9, further comprising fractionating or purifying the biological sample so that the sample contains a subset of the metabolites contained in the cell from which the sample is derived.

11. The method of any one of claims 1 to 10, wherein the metabolites are quantitatively determined by mass spectrometry.

12. The method of claim 11, wherein mass spectrometry is MALDI-TOF.

13. The method of any one of claims 1 to 12, wherein the metabolites are chromatographically separated prior to quantitative determination.

14. The method of any one of claims 1 to 13, further comprising the step of introducing external standards for one or more of the quantitatively determined metabolites.

15. The method of any one of claims 1 to 14, further comprising the step of identifying one or more of the metabolites which are quantitatively determined.

16. The method of claim 15, wherein said metabolites are identified by secondary fragmentation.

17. The method of claim 16, wherein identifying of said metabolites comprises electron impact ionisation, MS-MS technology and/or post source decay analyses of molecular ions or fragments.

18. The method of any one of claims 1 to 17, wherein said cell has been maintained under conditions additionally allowing the uptake of an isotopically unlabeled metabolizable compound and said compound and/or metabolic products thereof are quantitatively determined.

19. The method of claim 18, wherein the amount determined for the isotopically unlabeled metabolizable compound and/or said metabolic products thereof is compared with the amount obtained by carrying out said method correspondingly, but without the uptake of said unlabeled metabolizable compound.

20. The method of any one of claims 1 to 19, wherein, in addition to metabolites, one or more proteins and/or transcripts in said sample(s) is/are quantitatively determined and analysed.

21. The method of claim 20, wherein said metabolites and proteins and/or transcripts are each determined from the same biological sample.

22. The method of any one of claims 1 to 21, wherein said analysing further involves suitable statistical evaluation and correlation analyses of the data obtained and, optionally, network analyses.

23. A set of isotopically labeled metabolites obtainable from a sample which comprises or is derived from a cell which has been maintained under conditions allowing the uptake of an isotopically labeled metabolizable

compound so that the metabolites in said cell are saturated with the isotope with which said metabolizable compound is labeled.

24. Use of the set of isotopically labeled metabolites of claim 23 as a quantitative standard for determining the amount of one or more metabolites in a biological sample.

25. A kit comprising an isotopically labeled metabolizable compound and a manual for use in carrying in out the method of any one of claims 1 to 22 or the set of isotopically labeled metabolites of claim 23.

26. Use of an isotopically labeled compound that can be metabolized by a cell for labeling the metabolites in said cell in a saturating manner.

27. Use of an isotopically labeled compound that can be metabolized by a cell for the quantitative determination of metabolites in a biological sample comprising or being derived from said cell.

28. Use of an isotopically labeled compound that can be metabolized by a cell for analysing the metabolite profile of a biological sample comprising or being derived from said cell.

Figure 1

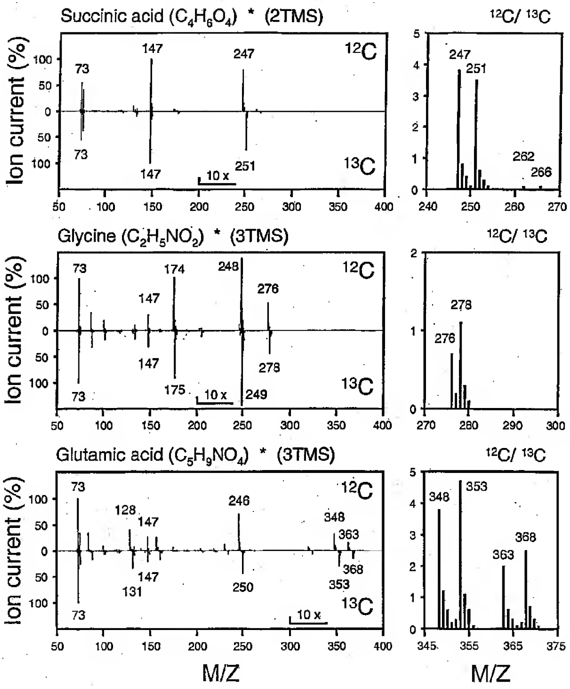

Succinic acid ($C_4H_6O_4$) * (2TMS)
Glycine ($C_2H_5NO_2$) * (3TMS)
Glutamic acid ($C_5H_9NO_4$) * (3TMS)
^{12}C/ ^{13}C
^{12}C
^{13}C
Ion current (%)
10 x
M/Z

Figure 2B

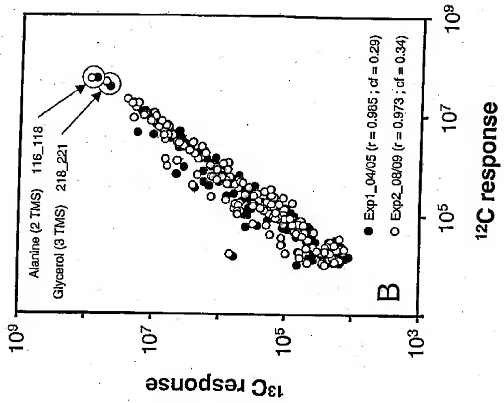


Figure 2A

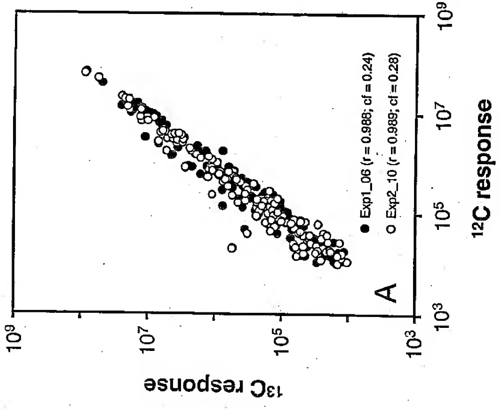


Figure 2C

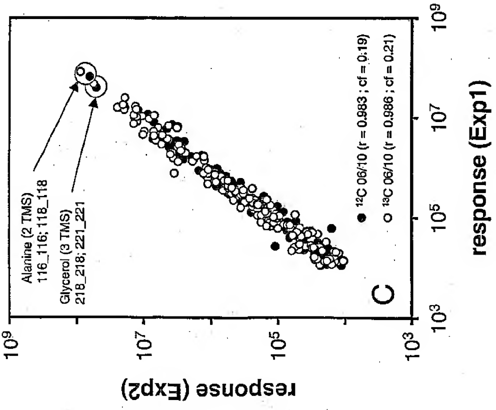
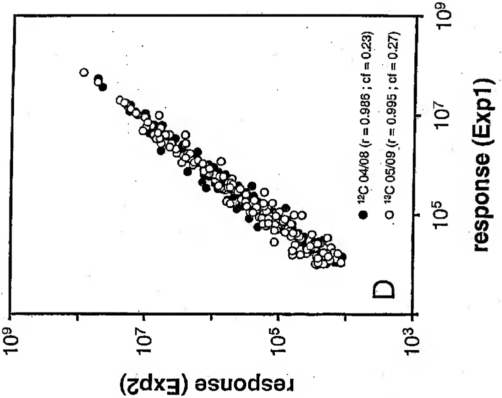


Figure 2D



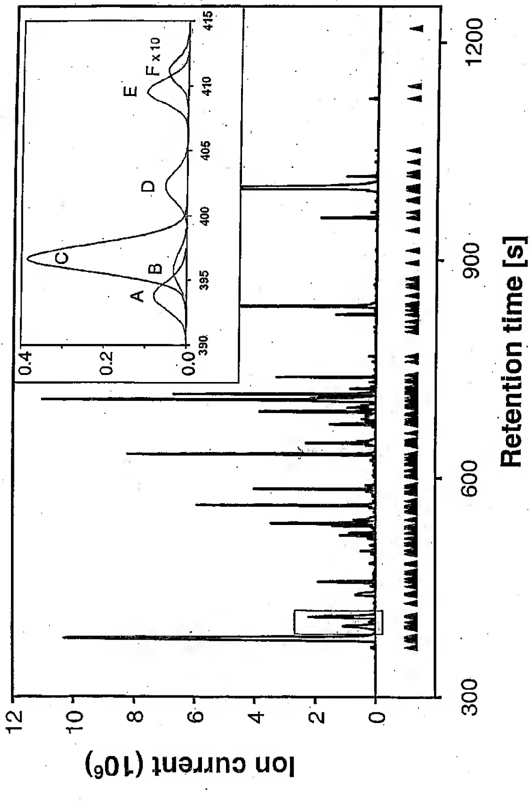

Ion current (10^6)
Retention time [s]
0
2
4
6
8
10
12
300
600
900
1200
0.0
0.2
0.4
390
395
400
405
410
415
A
B
C
D
E
F x 10

Figure 3

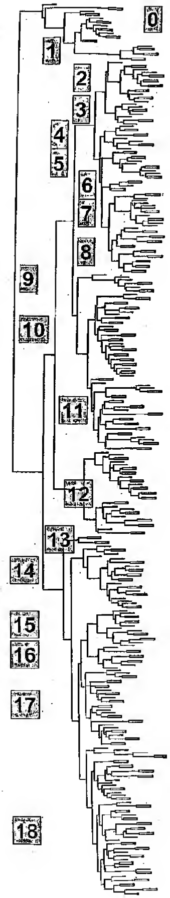


Figure 4A

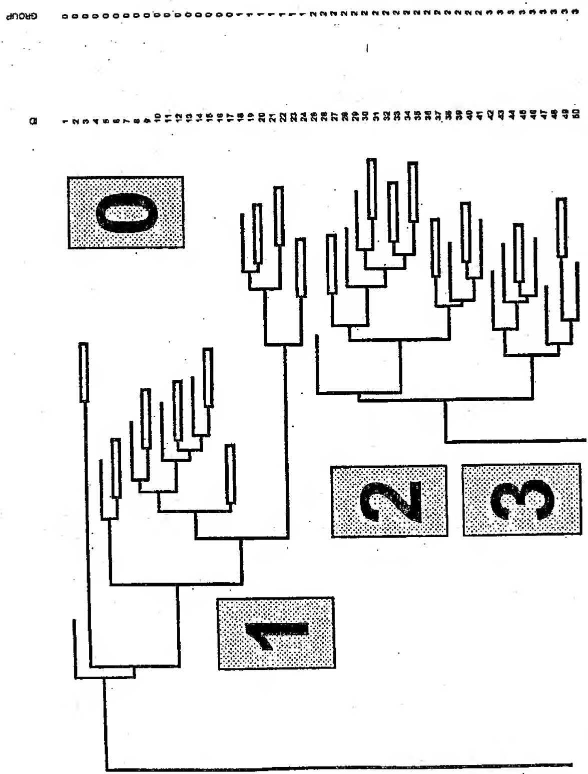


Figure 4B

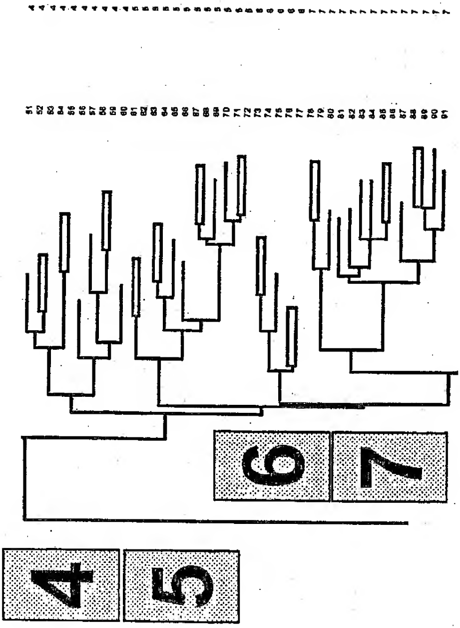


Figure 4C

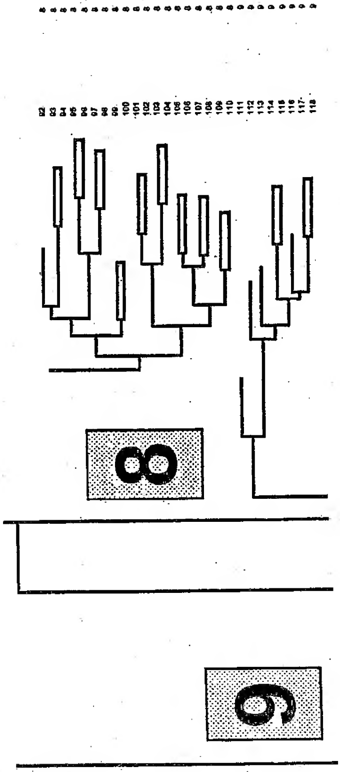


Figure 4D

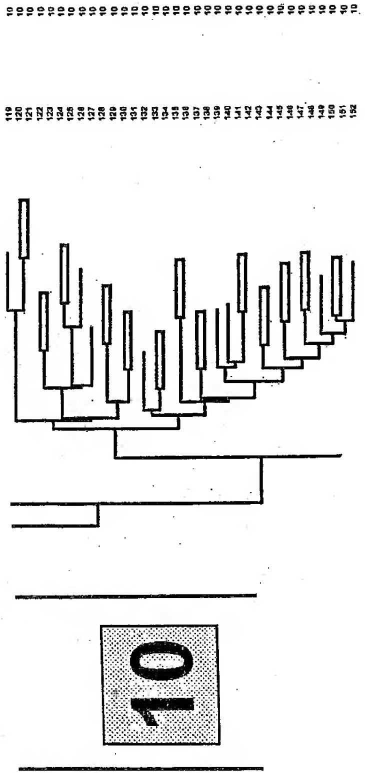
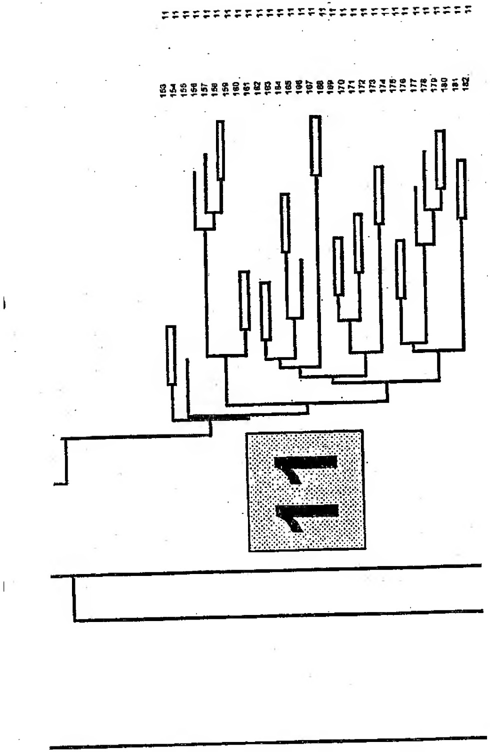


Figure 4E


153
154
155
156
157
158
159
160
161
162
163
164
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181
182

Figure 4F

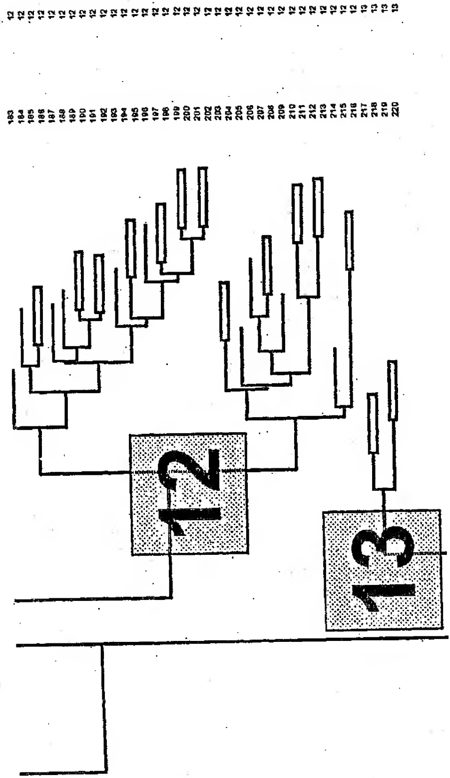


Figure 4G

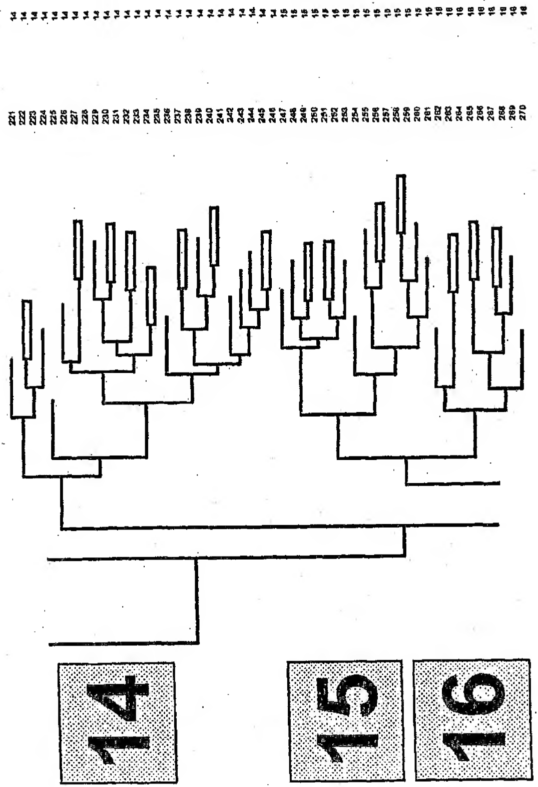


Figure 4H

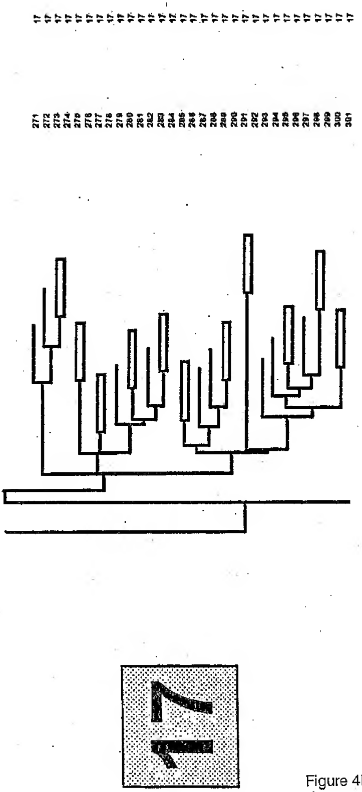


Figure 4l

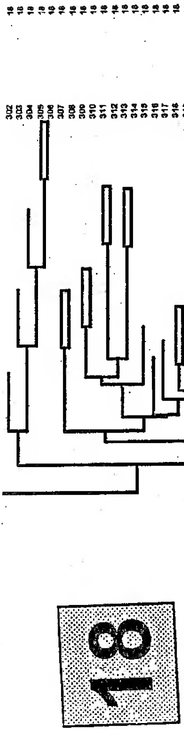


Figure 4J

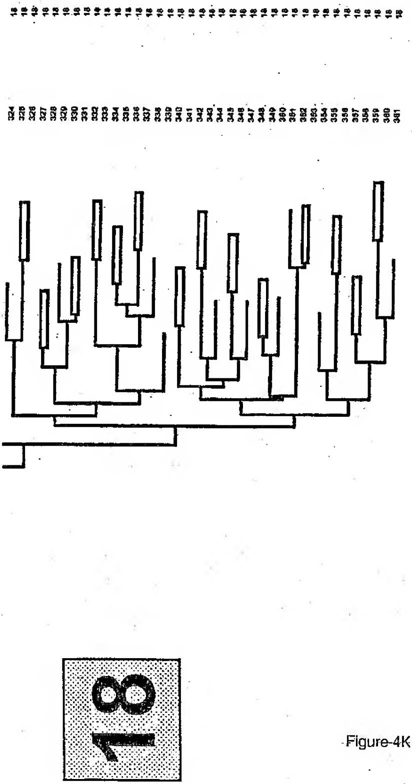


Figure-4K

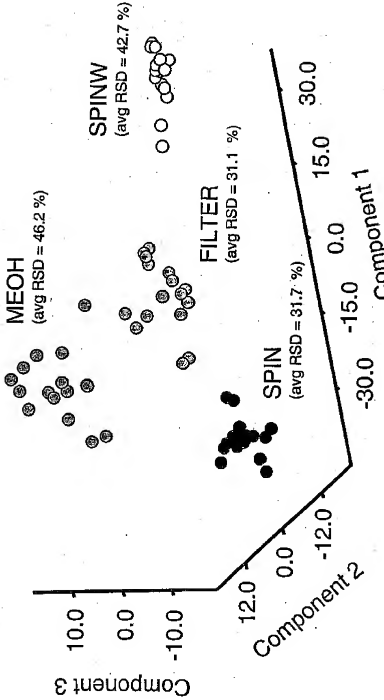

SPINW
(avg RSD = 42.7 %)
MEOH
(avg RSD = 46.2 %)
FILTER
(avg RSD = 31.1 %)
SPIN
(avg RSD = 31.7 %)
30.0
15.0
0.0
-15.0
-30.0
Component 1
12.0
0.0
-12.0
Component 2
10.0
0.0
-10.0
Component 3

Figure 5

Figure 6

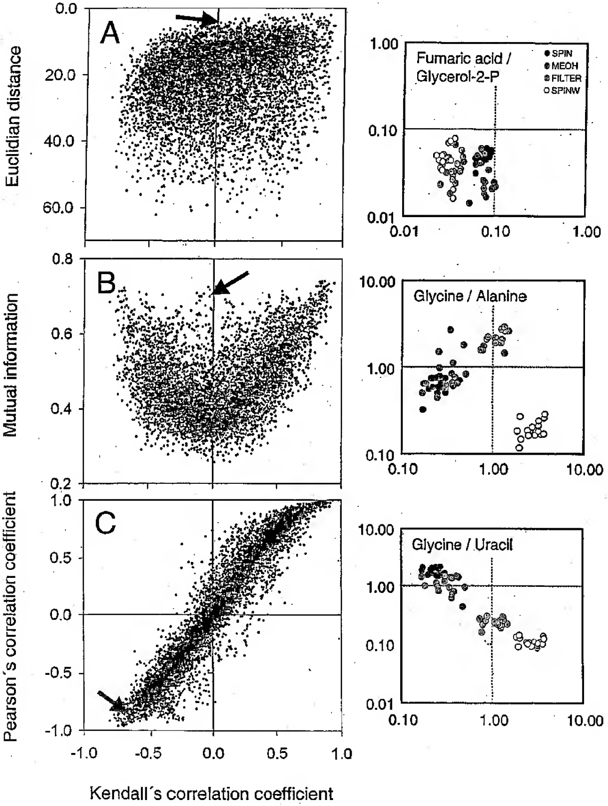

A
B
C
Euclidian distance
Mutual information
Pearson´s correlation coefficient
Kendall´s correlation coefficient
Fumaric acid / Glycerol-2-P
SPIN
MEOH
FILTER
SPINW
Glycine / Alanine
Glycine / Uracil

Figure 7

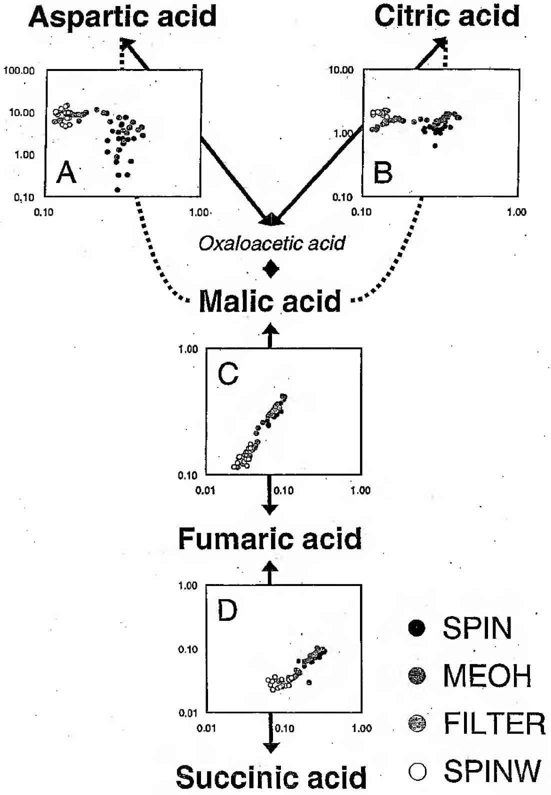

Aspartic acid
Citric acid
100.00
10.00
1.00
0.10
0.10
1.00
A
10.00
1.00
0.10
0.10
1.00
B
Oxaloacetic acid
Malic acid
1.00
0.10
0.01
0.10
1.00
C
Fumaric acid
1.00
0.10
0.01
0.01
0.10
1.00
D
Succinic acid
SPIN
MEOH
FILTER
SPINW

Figure 8

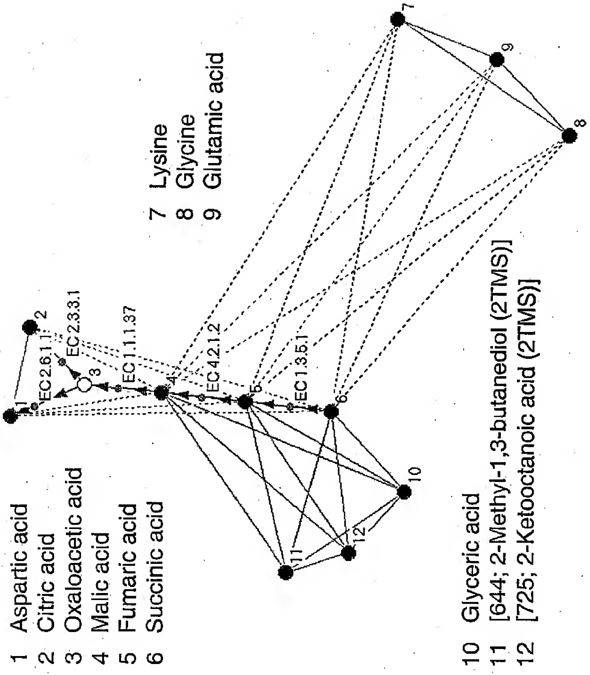
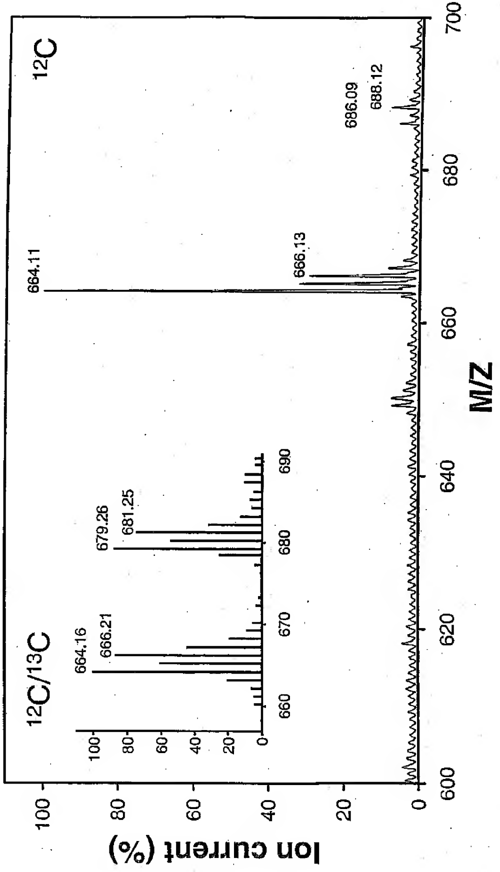

1 Aspartic acid
2 Citric acid
3 Oxaloacetic acid
4 Malic acid
5 Fumaric acid
6 Succinic acid
7 Lysine
8 Glycine
9 Glutamic acid
10 Glyceric acid
11 [644; 2-Methyl-1,3-butanediol (2TMS)]
12 [725; 2-Ketooctanoic acid (2TMS)]
EC 2.6.1.1
EC 2.3.3.1
EC 1.1.1.37
EC 4.2.1.2
EC 1.3.5.1

Figure 9


Ion current (%)
M/Z
12C
12C/13C
664.11
666.13
686.09
688.12
664.16
666.21
679.26
681.25
0
20
40
60
80
100
600
620
640
660
680
700
660
670
680
690

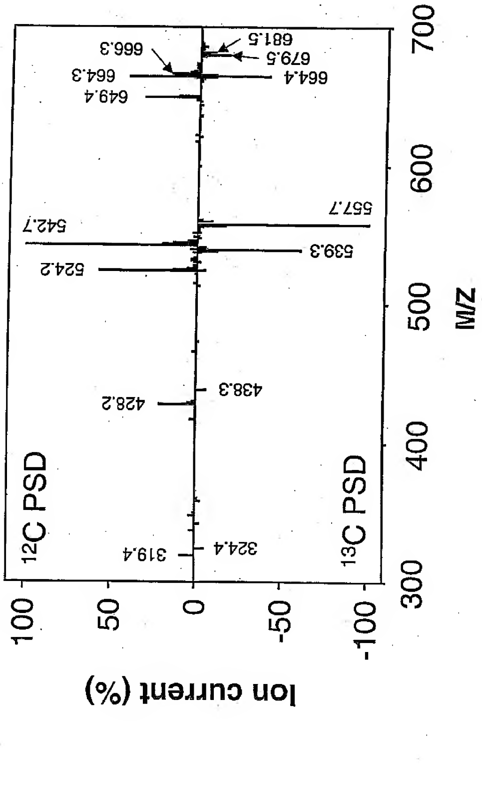

12C PSD
13C PSD
319.4
324.4
428.2
438.3
524.2
539.3
542.7
557.7
649.4
664.3
664.4
666.3
679.5
681.5
100
50
0
-50
-100
Ion current (%)
300
400
500
600
700
M/Z

Figure 10